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Methods for molecular mechanics modeling of coordination compounds

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CONTENTS

A. INTRODUCTION

(i) Scope and limitations of this review

This review focuses on the development of molecular mechanics (MM) models for molecules found in coordination chemistry, primarily the complexes of a single metal ion with organic ligands bearing oxygen, sulfur, nitrogen, or phosphorus donor atoms. MM calculations on such coordination compounds are based upon the extension of molecular models that were originally developed for the conformational analysis of organic compounds. Most of the current MM codes are capable of performing calculations on organic systems with a minimal level of input from the user. This capability has not yet been achieved with coordination compounds.

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Problems arise due to the variety of geometries that can occur at metal centers and the lack of parameters for interactions involving metal ions. This review analyzes the nature of these problems and the various methods that have been invented to solve them.

Several prior reviews have been written concerning the application of MM models to organic compounds [1–6] and the application of MM models to coordination compounds [7,8]. Reviews which the author has found most useful are listed below with a summary of their major areas of emphasis.

(1) N.L. Allinger, Calculation of molecular structure and energy by force-field methods, 1976 [3]. This article (253 references) provides a good general overview of the MM model and its application to organic compounds. Topics of discussion include force field development, energy minimization, and a review of the performance of MM models on different classes of organic compounds.

(2) S.R. Niketic and K. Rasmussen, The Consistent Force Field: A Documentation, 1977 [5]. This book (211 pages) provides a technical narrative on the inner organization of a MM code. Chapters cover topics such as molecular topology and geometry, conformational energy and potential functions, energy minimization methods, the optimization of parameter sets, and the development of force fields. Discussion includes applications to both organic compounds and coordination compounds, e.g. octahedral polyamine metal complexes.

(3) U. Burkert and N.L. Allinger, Molecular Mechanics, 1982 [4]. This book (339 pages) provides a detailed description of the basic principles and techniques of MM as applied to organic compounds. It includes an extensive compilation of reported MM calculations on organic compounds. This compilation is organized by functional group, starting with alkanes and proceeding through compounds that contain various heteroatoms. Discussion concerning coordination compounds is limited to two pages on the conformational analysis of several polyamine complexes of cobalt(III).

(4) G.R. Brubaker and D.W. Johnson, Molecular mechanics calculations in coordination chemistry, 1984 [7]. This article (80 references) reviews the application of MM calculations to the conformational analysis of polyamine and amino acid complexes of the cobalt(III) ion. Numerous examples are given where calculated structure and strain energies are related to experimental isomer distributions, thermodynamic stability, and kinetic stability.

(5) K. Rasmussen, Potential Functions in Conformational Analysis, 1985 [6]. This book (232 pages) begins with a review of the various types of force field and MM codes. This is followed by several chapters concerning the applications of these codes to several classes of compounds. One of these chapters contains a brief overview of calculations with coordination complexes. Subsequent chapters present examples and advice on the selection of potential functions and methods for their parameterization.

(6) R.D. Hancock, Molecular mechanics calculations as a tool in coordination chemistry, 1991 [8]. This article (128 references) reviews a variety of ways in which MM calculations have been used to understand factors controlling chelation. Topics that are addressed include the preference of metal ions for five- and six-membered chelate rings, the influence of steric strain upon complex stability, the conformational analysis of macrocyclic ligands, and the quantitative analysis of size-match selectivity.

With respect to coordination chemistry, prior reviews have tended to focus on how MM models are utilized, rather than how they are developed. They address such topics as how MM models have been applied in conformational analysis, how well the models can reproduce known structure, and how calculated structure and strain energies have been correlated with known thermodynamic and kinetic stabilities. Details presented on how to actually perform an MM calculation on a metal complex have been limited. These details include the types of potential energy equations, the development of force fields, and the MM codes that have been used to perform calculations on metal complexes.

The present review is intended to complement the prior ones by discussing issues related to the development of MM models for coordination compounds. Section A presents a brief review of the basic principles of MM. Section B contains a description of the types of potential energy equations that have been successfully applied to coordination compounds. The codes that have been used to implement these potential energy equations are identified. Methods used to develop parameters are also discussed. Section C provides a comprehensive compilation of reported MM calculations on coordination compounds.

(ii) Basic principles of molecular mechanics

Molecular mechanics (MM) models are used for conformational analysis, i.e. they are used to determine (i) which conformations are stable, (ii) which conformations are the most preferred, and (iii) the energy differences between stable conformations. To accomplish this, MM codes must generate an equation for each molecule that relates its potential energy to its nuclear coordinates. This equation defines a potential energy hypersurface of $3N + 1$ dimensions where $3N$ dimensions are used to specify the position of each of the N atoms in the molecule and the extra dimension specifies the potential energy. Each point on the potential surface corresponds to a geometry of the molecule. Minima on the potential surface correspond to stable conformations of the molecule. MM codes are able to locate these minima and, thereby identify stable conformations. The potential energy associated with each stable conformation is used to assign their relative stability.

In MM models, the equation that relates a molecule's potential energy to its conformation is composed of a sum of terms that represent different types of energy contributions. The types of term that are included in a potential energy equation often differs from one MM model to the next. In the simplest models, the total potential energy is broken down into four components:

$$U_{\text{total}} = \sum U_r + \sum U_\theta + \sum U_\phi + \sum U_{\text{vdw}} \tag{1}$$

The sums represent contributions to the total potential energy, U_{total}, due to bond stretching and compression terms, U_r, valence angle bending terms, U_θ, internal rotational or torsional terms, U_ϕ, and van der Waals interactions, U_{vdw}. In practice, other terms are sometimes added to the sum. These include electrostatic terms, improper torsion or out-of-plane bending terms, and cross-terms such as stretch–bend terms [4,5]. During a calculation, MM codes set the number of terms in the potential energy equation such that there is a term that corresponds to each bond, valence angle, torsion angle, and van der Waals atom pair in the molecule. Thus, the potential energy equation, U_{total}, is uniquely defined for each molecule.

The potential energies that are calculated by MM models are frequently identified by other names. These include internal energy, conformational energy, steric energy, and strain energy. This energy is defined relative to a hypothetical zero energy geometry that is unique to each molecule. This hypothetical geometry would be obtained if all bonds were at their equilibrium or stain-free length, all valence angles were at their equilibrium or stain-free angle, all torsional angles were in their lowest energy angle, and all van der Waals pairs were infinitely separated from one another. Note that this definition implies that negative strain energies are possible if contributions from attractive van der Waals forces are sufficiently large. Molecules are strained when their structural features (bond lengths, bond angles, torsion angles, van der Waals contacts) deviate from these zero energy values as defined by the potential functions. The zero energy geometry cannot be attained for most molecules and, therefore, MM models find most molecules to be strained to some extent, even when in their lowest energy conformation.

The terms in the potential energy equation are described by simple analytical expressions with adjustable parameters. These are called potential functions. Together, a set of potential functions and its corresponding set of parameters are called a force field. Force fields are categorized by the type of potential functions that they contain. The different kinds of organic MM force fields are discussed in detail elsewhere [1–6]. In this review, discussion will be limited to the two types of organic MM force field that have been applied to coordination compounds. These are valence force fields and extended valence force fields.

In a valence force field, all coupling between the bond lengths, bond angles, and torsional angles is neglected. The contributions to the potential energy equation are usually separated into bond stretching, angle bending, bond rotation, and van der Waals interactions as shown previously (eqn. (1)). The potential energy equations of extended valence force fields contain additional terms, called cross-terms, that couple the various degrees of freedom. For example, in such force fields a distortion in bond angle is usually coupled with the stretching of the bonds that form the angle. In general, cross-terms are added to improve the performance of organic force fields with severely strained molecules such as cyclobutane. Where extended valence force fields have been applied to coordination compounds, the cross-terms for interactions that involve the metal ion are generally omitted.

The mathematical form of the set of potential functions that are used in a potential energy equation varies from one MM code to the next. There are, however, certain potential functions that are routinely used to represent the various types of term in organic force fields [4–6]. For example, the potential energy equation usually contains a bond deformation term for each bond in the molecule. Harmonic potentials are commonly used to describe the change in potential energy that accompanies bond stretching and compression:

$$U_r = f_r \cdot (1/2)K_r \cdot (r - r_0)^2 \tag{2}$$

where r is the bond length, r_0 is the strain-free bond length, K_r is the force constant, and f_r is a unit conversion factor. Typically, lengths are in units of Å, K_r is in units of mdyn Å^{-1}, and f_r is assigned a value of 143.88 to give U_r in kcal mol^{-1}. The quantities r_0 and K_r are adjustable parameters that are assigned to each type of bond. In general, values for K_r that are used in organic force fields are sufficiently high for bond lengths not to vary significantly.

Harmonic potentials are only good approximations for small deformations in bond length. They are not suitable for use in molecules that contain highly strained bonds and they cannot be used to model the potential surface for bond dissociation. Alternative forms of the bond length deformation potential have been applied to include anharmonicity. Examples are the cubic equation (eqn. (3)) and the Morse function (eqn. (4)).

$$U_r = f_r \cdot (1/2)K_{r,1} \cdot (r - r_0)^2 \cdot [1 + K_{r,2} \cdot (r - r_0)] \tag{3}$$

$$U_r = D \cdot \{\exp[-2\alpha \cdot (r - r_0)] - 2 \cdot \exp[-\alpha \cdot (r - r_0)]\} \tag{4}$$

The potential energy equation usually contains a bending term for each bond angle in the molecule. The energy contributions from deformations of bond angles are also commonly treated with harmonic potential functions:

$$U_\theta = f_\theta \cdot (1/2)K_\theta \cdot (\theta - \theta_0)^2 \tag{5}$$

where θ is the bond angle, θ_0 is the strain-free bond angle, K_θ is the bending force constant, and f_θ is a unit conversion factor. The quantities θ_0 and K_θ are the adjustable parameters in this potential function. Typically, bond angles are in units of degrees, K_θ is in units of mdyn · Å rad^{-2}, and f_θ is assigned a value of 0.043828 to give U_θ in kcal mol^{-1}. The quantities θ_0 and K_θ are adjustable parameters that are assigned to each type of bond angle. The values of K_θ that are used in organic force fields are roughly a tenth the magnitude of the bond stretching force constants. Therefore, the model allows bond angles to be more easily distorted.

As with bond length deformations, harmonic bending potentials do not adequately describe large deformations in bond angle. Some codes employ higher-order polynomials to include some anharmonicity in the bending potential functions, for example:

$$U_\theta = f_\theta \cdot (1/2)K_{\theta,1} \cdot (\theta - \theta_0)^2 \cdot [1 + K_{\theta,2} \cdot (\theta - \theta_0)^4] \tag{6}$$

Extended valence force fields couple bond stretching with bond angle deformation by including stretch–bend terms. A typical stretch–bend potential function is

$$U_{r,\theta} = f_{r,\theta} \cdot (1/2)K_{r,\theta} \cdot (r - r_0) \cdot (\theta - \theta_0) \tag{7}$$

where r and θ are the bond length and bond angle, r_0 and θ_0 are the same strain-free lengths and angles that are used in the bond stretching and bond angle potentials, $K_{r,\theta}$ is the stretch-bend force constant, and $f_{r,\theta}$ is the unit conversion factor. Typically, bond lengths are in units of Å, bond angles are in units of degrees, $K_{r,\theta}$ is in units of mdyn rad^{-1}, and $f_{r,\theta}$ is assigned a value of 2.5112 to give $U_{r,\theta}$ in kcal mol^{-1}. These terms generally do not represent a significant contribution to the overall potential energy unless the molecule is highly strained.

Torsional energy terms are added to the potential energy equation in order to obtain the correct barriers to rotation about bonds. The general form of the potential function that is used to describe torsional energy is a Fourier series expansion of the torsional angle:

$$U_\phi = \sum (1/2)V_n \cdot [1 + s \cdot \cos(n \cdot \phi)] \tag{8}$$

where ϕ is the torsional angle that is allowed to vary from 0 to 360°, V_n is the effective barrier to rotation, s is either $+1$ or -1 depending on whether the eclipsed conformation ($\phi = 0°$) is a maximum or a minimum on the potential surface, and n is the periodicity of the barrier. Typically, torsional angles are in units of degrees and V_n is in units of kcal mol^{-1} to give U_ϕ in kcal mol^{-1}. The quantities V_n, s, and n are adjustable parameters that are assigned to each type of torsion. Since van der Waals terms also contribute to the calculated rotational barriers, the values that are used for V_n are lower than experimental rotational barriers.

It is common practice in many force fields to use only one term of the Fourier series when describing rotations about organic bonds. For example, the torsional potential function for the C–C single bond in ethane reduces to

$$U_\phi = (1/2)V_3 \cdot [1 + \cos(3 \cdot \phi)] \tag{9}$$

and the torsional potential function for the C=C double bond in ethylene reduces to

$$U_\phi = (1/2)V_2 \cdot [1 - \cos(2 \cdot \phi)] \tag{10}$$

Other force fields use combinations of the first three terms in the Fourier series to describe these torsions. Codes also differ in the way that they implement the torsional potential function. Some codes consider only one torsional angle per bond. Other codes consider all combinations of outer pairs of atoms and sum over all contributions for each bond. In the latter case, ethane would require a total of nine terms, one for each of the nine H—C—C—H torsion angles.

Another type of term that is often included in the potential energy equation is an out-of-plane bending term or improper torsion. This term is added to account for the energy contribution arising from the out-of-plane deformation of sp^2 hybridized atoms. A simple potential function that is used to describe this energy is

$$U_{\mathrm{opb}} = f_{\mathrm{opb}} \cdot K_{\mathrm{opb}} \cdot \delta^2 \tag{11}$$

where δ is the distance of the sp^2 atom from the plane defined by the three attached atoms, K_{opb} is the out-of-plane force constant, and f_{opb} is a unit conversion factor. Typically, distance is in units of Å, K_{opb} is in units of mdyn Å^{-1}, and f_{opb} is assigned a value of 143.88 to give U_r in kcal mol^{-1}. The quantity K_{opb} is an adjustable parameter that is assigned to each type of sp^2 atom.

Extended valence force fields couple bond stretching with bond rotation by including stretch–torsion terms. An example of a stretch–torsion potential function is

$$U_{r,\phi} = f_{r,\phi} \cdot (1/2) K_{r,\phi} \cdot (r - r_0) \cdot [1 + \cos(3\phi)] \tag{12}$$

where r and ϕ are the bond length and torsion angle, r_0 is the same strain-free length that is used in the bond stretching potential, $K_{r,\phi}$ is the stretch–bend force constant, and $f_{r,\phi}$ is the unit conversion factor. Typically, bond lengths are in units of Å, torsion angles are in units of degrees, $K_{r,\phi}$ is in units of mdyn, and $f_{r,\phi}$ is assigned a value of 143.88 to give $U_{r,\phi}$ in kcal mol^{-1}. As with stretch–bend terms, stretch–torsion terms generally do not represent a significant contribution to the overall potential energy unless the molecule is highly strained.

The potential energy equation usually includes a van der Waals term for all atom pairs in the molecule that are neither bonded together nor attached to a common atom. The energy contributions from van der Waals interactions are commonly treated with one of two potential functions that give the van der Waals energy as a function of the distance, r, between the atoms. These are the Lennard–Jones potential function (eqn. (13)) and the modified Buckingham potential function (eqn. (14)):

$$U_{\mathrm{vdw}} = \frac{A}{r^{12}} - \frac{C}{r^6} \tag{13}$$

$$U_{\mathrm{vdw}} = A \cdot \exp(-B \cdot r) - \frac{C}{r^6} \tag{14}$$

Each of these functions contains an attractive term, $-C/r^6$, that dominates at large distances and a repulsive term, either A/r^{12} or $A \cdot \exp(-B \cdot r)$, that dominates at short distances. These expressions can be rewritten as

$$U_{\mathrm{vdw}} = \varepsilon \cdot \left(\frac{r^*}{r}\right)^{12} - 2 \cdot \varepsilon \cdot \left(\frac{r^*}{r}\right)^{6} \tag{15}$$

$$U_{\mathrm{vdw}} = \frac{\varepsilon}{(1-(6/\alpha))} \cdot \left[\frac{6}{\alpha} \cdot \exp\left\{\alpha \cdot \left(1 - \frac{r}{r^*}\right)\right\} - \left(\frac{r^*}{r}\right)^{6}\right] \tag{16}$$

where r^* is the most stable interatomic distance in terms of potential energy for the pair of atoms, ε is the work required to separate the two atoms to infinity, and α is a dimensionless parameter that controls the steepness of the exponential repulsion term. Some codes use one of the forms in eqns. (13) or (14) and assign individual sets of parameters (A and C or A, B, and C) of each type of atom pair. Other codes use one of the forms in eqns. (15) or (16), and it is assumed that r^* is the sum of the van der Waals radii for the two atoms and ε is the geometric mean of the value for identical pairs of the different atoms, i.e. $\varepsilon_{ij} = (\varepsilon_i \cdot \varepsilon_j)^{1/2}$. The latter approach requires fewer parameters, two per atom type rather than two or three per each type of atom pair. Typically, r and r^* are in units of Å, and ε is in units of kcal mol^{-1} to give U_{vdw} in kcal mol^{-1}.

A potential energy equation may also contain terms for the energy contributions that are attributed to electrostatic interactions. The approach used to treat these interactions varies. Some codes implement a point charge model and use the familiar Coulomb expression

$$U_{\mathrm{el}} = \frac{f_{\mathrm{el}} \cdot q_i \cdot q_j}{\varepsilon \cdot r} \tag{17}$$

where r is the distance separating the charges, q_i and q_j are point charges, ε is the effective dielectric constant, and f_{el} is a unit conversion factor. The interactions may be summed over all possible pairs of charged atoms or, as with the van der Waals interactions, limited to charged atom pairs that are neither attached to one another nor to a common atom. Typically, r is in units of Å, and f_{el} is assigned a value of 332.07 to give U_{el} in kcal mol^{-1}. As with the van der Waals interactions, the potential energy equation will usually include coulombic terms only for the pairs of charged atoms that are neither bonded together nor bonded to a common atom.

Other codes model electrostatic contributions as the interaction between dipoles within the molecule. A term is added to the potential energy equation for all pairs of dipoles that are not attached to the same atom. The potential function used to describe the energy that results from the interaction of two dipoles is

$$U_{\mathrm{el}} = \frac{f_{\mathrm{el}} \cdot \mu_i \cdot \mu_j}{(\varepsilon \cdot r^3)} [\cos X - \cos \alpha_i \cdot \cos \alpha_j] \tag{18}$$

where μ_i and μ_j are the bond moments, ε is the effective dielectric constant, r is the distance between the mid-points of the bonds, X is the angle between the dipoles, α_i

and α_j are the angles between the dipole axes and the line along which r is measured, and f_{el} is a unit conversion factor. Typically, r is in units of Å, μ is in units of Debye, ε is dimensionless, angles are in degrees, and f_{el} is assigned a value to 14.394 to give U_{el} in kcal mol^{-1}.

Such potential functions have been chosen for use in MM force fields because the shape of the potential surfaces that they generate correspond to accepted chemical ideas about the nature of forces acting in a molecule, they are simple enough to allow for speed in computing, the number of adjustable parameters they require is minimal, and, perhaps most importantly, they have been found to yield transferable force fields [4,5]. Transferability is the fundamental basis for all MM models. Simply stated, transferability means that a potential function and parameters for any given interaction, e.g. a $C(sp^3)$–$C(sp^3)$ bond stretch, are applicable to that interaction regardless of the molecular environment in which the interaction is found. Because of this property, simple force fields equipped with relatively small parameter sets can be used to model a large number of molecules.

Force fields are developed to treat classes of compounds which are composed of the same atom types. Examples of classes of compounds include alkanes, amines, ethers, and so on. Once a class of compounds has been targeted, the first step in the development of a force field is to identify the types of term to be included in the potential energy equation. Potential functions are selected and assigned to these terms. The potential functions are parameterized such that the force field reproduces experimentally known structures and potential surfaces for a test set of molecules from the target class. It is important to use a large a set of molecules for the parameterization process in order to test the limits of the transferability of the force field. If the resulting force field performs adequately on the test set of molecules, then it is assumed that the model can be used to predict the properties of other molecules belonging to this class. If the force field cannot be parameterized to reproduce the properties of the molecules in the test set, then the potential energy equation is modified by altering the form of the potential functions or including additional terms, and the parameterization process is continued. The goal is to develop a force field with the simplest set of potential functions and least number of parameters that provides an accurate transferable MM model.

B. FORCE FIELDS FOR COORDINATION COMPOUNDS

At this time there are many MM codes available that contain force fields that have been developed to treat a wide range of organic compounds [6]. In contrast, the MM codes and force fields that have been developed for coordination compounds are very limited in the type of ligands and metal ions that can be treated. Therefore, those who conduct MM calculations on coordination compounds have had to and will continue to have to build the force fields needed for the work. Since the bulk of the structure in many coordination compounds is composed of organic constituents, the natural tendency has been to adapt existing organic force fields to allow the addition of a metal ion. In fact, all the calculations that have been done on coordination compounds have been done with extended organic MM codes. In this way it is not necessary to develop an entire new force field, but only the portion of the force field that is needed to treat the new interactions incurred by the presence of the metal ion. This process may be as simple as adding a few parameters to the force field or as complex as rewriting sections of the code.

This section reviews the techniques that have been developed to extend organic MM codes to coordination compounds. The first part is concerned with how the potential energy equations of organic force fields can be adapted to provide suitable potential surfaces for the structure found in metal complexes. The second part is concerned with the methods that are used to obtain the parameters for these potential energy equations.

(i) Potential energy equations

Many different organic MM codes have been adapted for calculations on coordination compounds. The organic force fields in these codes differ in the types of term that are included in the potential energy equations, in the form of their potential energy functions, and in their parameter sets. Yet, despite this variation, only a few methods have evolved to extend them to treat metal complexes. These methods differ in the type of terms that are added to the potential energy equation to describe the interactions that involve the metal ion.

Descriptions of these methods are presented below. The merits and faults of each method are discussed with respect to its ease of implementation and its flexibility in handling the variety of geometries that occur at metal centers. Codes that have been used to implement these methods in reported calculations on coordination compounds are identified. For illustrative purposes, it will also be shown how each method would be implemented to extend a representative organic MM code to the octahedral complex $M(NH_2CH_3)_6$.

The representative organic MM code is based on the potential energy equation given in eqn. (19). It contains a default parameter set that contains all the parameters needed to model the organic portion of the complex, i.e. the NH_2CH_3 ligands. Like most organic MM codes, it is limited to four attachments per atom. In normal operation, the code will generate a potential energy equation with a term for each bond, a term for each bond angle, a term for each torsion angle, and a term for all non-bonded interactions involving atom pairs that are not connected to one another or to a common atom.

$$\begin{aligned} U_{\text{total}} = {} & f_r \cdot \sum (1/2) K_r \cdot (r - r_0)^2 + f_\theta \cdot \sum (1/2) K_\theta \cdot (\theta - \theta_0)^2 \\ & + \sum (1/2) V \cdot (1 + s \cdot \cos(n \cdot \phi)) \\ & + \sum A \cdot \exp(-B \cdot r) - (C/r^6) + f_{\text{el}} \cdot \sum q_1 \cdot q_2 / (\varepsilon \cdot r) \end{aligned} \tag{19}$$

(a) Valence force field method

The valence force field or VFF method is the most commonly used approach [9–108]. It is based upon the logical extension of an organic valence force field, i.e. the metal ion is treated like any other atom in an organic molecule. In theory, this means that terms are added to the potential energy equation for each M—L bond, M—L—X angle, L—M—L angle, M—L—X—X torsion, L—M—L—X torsion, and each M··X non-bonded interaction (M = metal ion, L = ligand donor atom, X = any other atom type). In practice, however, several of these terms are usually omitted from the potential energy equation.

The terms that are usually omitted include the L—M—L—X torsions, M··X van der Waals interactions, and M··X electrostatic interactions. The L—M—L—X torsional terms are omitted because the rotational barriers about M—L bonds are, in general, very low [5,14]. It has not been necessary to include them to obtain transferable force fields. Similarly, VFF calculations that have been conducted with and without the M··X non-bonded interactions present have shown that the addition of these terms does not significantly change the final conformations and relative energies that are obtained [71,72,84]. This is not surprising when one considers that, due to the way that non-bonded interactions are normally assigned, both van der Waals and electrostatic interactions with the metal ion are limited to atoms separated from the metal ion by three or more bonds.

It is a relatively simple matter to adapt the representative MM code to apply the VFF method to $M(NH_2CH_3)_6$. The code must first be modified to allow for an increased number of attachments per atom. In addition, it is necessary to make some provision for the fact that there are two types of N—M—N angle in this complex, cis and trans. This provision is necessary because organic MM codes normally assign parameters to potential functions based solely upon the atom types that are involved. Without some additional modification, the code would not distinguish between the two types of N—M—N angle. Finally, the terms for the L—M—L—X torsions and M··X non-bonded interactions are removed by assigning appropriate parameters for these interactions. This can be done by setting the barrier for rotation about M—L bonds to zero, setting the van der Waals parameters A and C for all M··X interactions to zero, and assigning a zero charge to the metal ion. With these modifications, the code now includes the following metal-dependent terms in the potential energy equation:

No. of terms		Interaction	Potential function	No. of parameters
6	×	M—N stretch	$f_r \cdot (1/2)K_r \cdot (r - r_0)^2$	2
12	×	*cis*-N—M—N bend	$f_\theta \cdot (1/2)K_\theta \cdot (\theta - \theta_0)^2$	2
3	×	*trans*-N—M—N bend	$f_\theta \cdot (1/2)K_\theta \cdot (\theta - \theta_0)^2$	2
12	×	M—N—H bend	$f_\theta \cdot (1/2)K_\theta \cdot (\theta - \theta_0)^2$	2
6	×	M—N—C bend	$f_\theta \cdot (1/2)K_\theta \cdot (\theta - \theta_0)^2$	2
18	×	M—N—C—H torsion	$(1/2)V \cdot [1 + \cos(3 \cdot \phi)]$	1

This is a total of 57 terms that will use 11 parameters. The first six terms define the M—N bond length preference, the next 15 terms define the N—M—N bond angle preference, and the remaining terms define preferences for the orientation of the ligand relative to the metal ion.

The problem of properly assigning multiple ideal angles at an atom center does not occur in organic molecules where geometries are limited to linear (one 180° angle), trigonal planar (three 120° angles), and tetrahedral (six 109.5° angles) arrangements. On the other hand, with the exception of the tetrahedral geometry, this problem occurs with all of the common geometries that are found at metal centers. These include square planar (six angles of two types), square pyramidal (ten angles of two types), trigonal bipyramidal (ten angles of three types), octahedral (15 angles of two types), trigonal prismatic (15 angles of three types), pentagonal bipyramidal (21 angles of three types), capped trigonal prismatic (21 angles of five types), capped octahedral (21 angles of four types), hexagonal bipyramidal (28 angles of three types), square antiprismatic (28 angles of four types) and dodecahedral (28 angles of five types) geometries. It can be seen that the problem of assigning ideal L—M—L angles becomes more difficult as the coordination number is increased.

Due to the difficulties associated with the assignment of preferred angles at the metal center, the VFF method is best suited for geometries with two or less L—M—L angle types, i.e. complexes with coordination numbers of $\leqslant 6$. Various solutions to the angle assignment problem have been devised. One option is to define each ligand donor atom as a different atom type and assign the appropriate ideal value to each of the individual angles. Another option is to alter the code such that all trans L—M—L bending interactions are omitted from the calculation. This approach is effective in treating square planar, square pyramidal, and octahedral geometries. A third option, which has only recently been developed [108], involves the definition of L—M—L angular preferences with respect to a spherical coordinate system.

The VFF method can be implemented in organic MM codes by adapting them to handle an increased number of attachments per atom and providing some mechanism to allow for the proper assignment of L—M—L angles. Codes that have been used to perform such calculations include Boyd's code and many modified versions of it [9–68], a modified version of the Wiberg program [69,70], the CFF program [71–82], several modified versions of the MM2 program [83–94], the AMBER program (coordination numbers of four) [95–98], a modified version of the MODEL program [99], the MacroMODEL program [100], the AGNAS program (coordination numbers of four) [101], the BIOGRAF program [102–104], the MOLMEC program [105,106], and a modified version of the CHARMM program [108]. Details on how to modify the MM2 program to implement the VFF method with metal complexes that contain up to six ligands have been reported [92].

(b) Points-on-a-sphere method

The points-on-a-sphere or POS method derives from a simple theory that has long been used to predict and rationalize the geometries found in coordination compounds [109–111]. This simple theory states that the donor atoms attached to a metal ion tend to distribute themselves in such a way as to minimize donor atom–donor atom repulsions. It has been demonstrated that most coordination geometries can be explained by merely considering the distribution of points on the surface of a sphere with an appropriate repulsive force between them [112–117].

In MM calculations that employ the POS method [69,118–144], the inner coordination sphere of the metal ion is treated in a similar fashion. Rather than define a set of L–M–L angles for each geometry, all L–M–L terms are replaced by L··L van der Waals terms. Thus, the POS method allows the L–M–L angles to be dictated by van der Waals interactions between the ligand donor atoms. All other metal-dependent interactions are treated exactly as in the VFF approach, i.e. terms for each M–L bond, M–L–X angle, and M–L–X–X torsion are added to the potential energy equation and, as before, terms for each L–M–L–X torsion and M··X non-bonded interaction are usually omitted from the potential energy equation.

To adapt the representative MM code to treat $M(NH_2CH_3)_6$ with the POS method, it is necessary to make several modifications. The allowed number of attachments per atom must be increased. All L–M–L interactions must be removed. This can be accomplished with a code modification or simply by setting all L–M–L bending force constants to zero. The L··L van der Waals terms, which normally would not be present, must be added to the potential energy equation. Finally, L–M–L–X torsions and M··X non-bonded interactions are removed as in the VFF method. With these modifications, the code will now include the following metal-dependent terms in the potential energy equation:

No. of terms		Interaction	Potential function	No. of parameters
6	×	M–N stretch	$f_r \cdot (1/2)K_r \cdot (r - r_0)^2$	2
15	×	N··N van der Waals	$A \cdot \exp(-B \cdot r) - (C/r^6)$	3
12	×	M–N–H bend	$f_\theta \cdot (1/2)K_\theta \cdot (\theta - \theta_0)^2$	2
6	×	M–N–C bend	$f_\theta \cdot (1/2)K_\theta \cdot (\theta - \theta_0)^2$	2
18	×	M–N–C–H torsion	$(1/2)V \cdot [1 + \cos(3 \cdot \phi)]$	1

This is a total of 57 terms that will use ten parameters. The first six terms define the M–N bond length preference, the next 15 terms define the N–M–N bond angle preference, and the remaining terms define preferences for the orientation of the ligand relative to the metal ion.

The POS method offers some decided advantages over the VFF method. Application of the POS method avoids the problematic definition of ideal L–M–L angles. In addition, it requires fewer parameters. Default van der Waals parameters from organic force fields are usually used for the L··L interactions. If default van der

Waals parameters are used for the N··N interactions in $M(NH_2CH_3)_6$, the POS method adds only seven new parameters, while the VFF method adds 11. Note that the difference between the two methods becomes more pronounced in geometries with more angle types and complexes that contain multiple donor atom types.

Potential energy surfaces that are generated by the POS method yield minima that correspond to most geometries that are encountered at metal centers [113–117]. An exception arises with four coordinate metal complexes where L··L repulsive forces alone always favor a tetrahedral arrangement. Thus, additional measures are required to obtain square planar geometries. Three methods that can be used for this purpose are (i) restricting the metal and the four donor atoms to lie in the same plane, (ii) placing lone pairs in the axial positions, and (iii) employing an out-of-plane bending term at the metal ion [120]. MM calculations based on the POS method have been used to calculate square planar [120,124,128,130,135–139], square prismatic [124,128,138], trigonal bipyramidal [139], octahedral [69,118–129,131–134], trigonal prismatic [139], capped trigonal prismatic [139–141], capped octahedral [139,141], and pentagonal bipyramidal geometries [139], as well as a number of geometries that occur with higher coordination numbers [142–144].

The POS method can be implemented in organic MM codes by adapting them to handle an increased number of attachments per atom and to replace L–M–L bending interactions with L··L van der Waals interactions. Codes that have been used to perform such calculations include a modified version of the Wiberg program [69], Boyd's program and several modified versions of it [118–127,142,143], the MOMEC program [128–138], and two modified versions of the MM2 program [139–141]. Recently, a technique has been reported that allows the POS method to be implemented with the MM2 program without requiring any modification to the code [144].

(c) Ionic method

The ionic method, also known as the pair potential method, is quite different from the preceding two methods. In the ionic method, the interaction of a metal ion with the ligand(s) is modeled entirely with M··L non-bonded terms [67,145–165]. All M··L and M··X van der Waals interactions and electrostatic interactions are included in the potential energy equation and all M–L, L–M–L, M–L–X, and M–L–X–X terms are omitted from the potential energy equation. Unlike the VFF and POS methods, structures and energies calculated with the ionic method are extremely sensitive to the charge and the van der Waals parameters that are assigned to the metal ion. This difference is due to the way that non-bonded terms are applied in the various methods. In the VFF and POS methods, M–L bonds are explicitly defined and non-bonded interactions involving the metal ion can only occur with atoms that are at least three bonds away. Such interactions do not usually have a significant impact on the results of the calculations and, as discussed earlier, they are typically omitted. In the ionic method, however, the metal ion is directly engaged in electrostatic and van der Waals interactions with all atoms of the ligands, and it is the balance between electrostatic and van der Waals forces alone that determines all aspects of the calculated structure.

The representative MM code does not require any modification to apply the ionic method to $M(NH_2CH_3)_6$. However, it is necessary that the starting structure be correctly defined. The metal ion is positioned in the center of an octahedral array of the ligands, but the metal ion is not connected to the donor atoms. This starting structure is such that the code will automatically include the following metal-dependent terms in the potential energy equation:

No. of terms		Interaction	Potential function	No. of parameters
6	×	M··N van der Waals	$A\cdot\exp(-B\cdot r)-(C/r^6)$	3
6	×	M··C van der Waals	$A\cdot\exp(-B\cdot r)-(C/r^6)$	3
30	×	M··H van der Waals	$A\cdot\exp(-B\cdot r)-(C/r^6)$	3
6	×	M··N electrostatic	$f_{el}\cdot q_1\cdot q_2/(\varepsilon\cdot r)$	2
6	×	M··C electrostatic	$f_{el}\cdot q_1\cdot q_2/(\varepsilon\cdot r)$	2
12	×	M··H (N̲H) electrostatic	$f_{el}\cdot q_1\cdot q_2/(\varepsilon\cdot r)$	2
18	×	M··H (C̲H) electrostatic	$f_{el}\cdot q_1\cdot q_2/(\varepsilon\cdot r)$	2

This is a total of 84 terms that will use 14 parameters (nine van der Waals parameters and five point charges). The M—L bond length preference is controlled by a balance of coulombic attractions and van der Waals repulsions between the metal cation and the negatively charged donor atoms, the L—M—L bond angle preference is dictated by non-bonded interactions between the ligands, and the M—L—X angles and M—L—X—X torsion angles result from a complex interplay of many pair-wise non-bonded interactions.

The ionic method offers several advantages over the other approaches. It is simple to implement with most organic MM codes. Like the POS method, the ionic method avoids the problems associated with the definition of ideal L—M—L angles and provides a potential surface that accommodates a variety of geometries at the metal center. Another advantage is that the ionic method yields a potential surface for M—L bond stretching that exhibits nearly harmonic behavior for small displacements from the equilibrium bond length, but also allows for M—L bond dissociation and, thus, allows for the coordination number to change during a calculation.

The simplicity of the ionic method can also be a disadvantage. While it is possible to parameterize the force field to reproduce M—L bond lengths, the omission of all the terms that are usually present in a valence force field may make it difficult to reproduce adequately other structural features such as L—M—L angles, M—L—X angles, and M—L—X—X torsional interactions. More than one group has found it necessary to add additional terms to the potential energy equation of an ionic model to control angular preferences at the metal center and orientation preferences of the ligand [150,162–165]. Due to a lack of data, the majority of the structures that have been calculated with the ionic method have not actually been compared with experimental structures. Therefore, it is not clear whether the ionic method provides an adequate potential surface for the accurate modeling of structure in metal complexes or whether the ionic method will yield transferable force fields.

The ionic method can be implemented with any organic MM code that supports the use of electrostatic terms that are based upon the interaction of point charges. Codes that have been used to perform such calculations include Boyd's program [67,150], the AMBER program [145–149], the YETI program [151,162–165], the WMIN program [152], the MMPP program [153,154], and the MM2 program [155].

(ii) Parameters

The preceding discussion has documented several ways that organic MM codes can be adapted for calculations on coordination compounds. After selecting a method and obtaining a code to implement it, one more task is required before modeling can be performed. This final task is the assignment of force field parameters. Most MM codes are equipped with a force field that already contains parameters for common organic functional groups. These force fields can be used to model many types of uncomplexed organic ligands. When modeling coordination compounds, it is generally assumed that the complexation of the ligand to a metal ion does not significantly alter the nature of the interactions within the ligand. In other words, the parameters that are used for modeling the ligand structure within a metal complex are assumed to be transferable from organic force fields. The validity of this assumption has been repeatedly supported by the successful outcome of numerous calculations on a wide variety of complexed ligands (see Scheme 1, below).

Since it is usually possible to use existing parameter sets for the interactions within the ligand, the most frequently adopted approach to parameterize a force field for a class of coordination compounds has been to select an organic force field and to add only those parameters that are needed for the interactions of the metal ion with the ligand. These metal-dependent parameters are obtained with the same techniques that are used for the development of organic parameter sets [1–6]. Experimental data are taken from a variety of independent sources to yield an initial set of parameters. The performance of this initial set is tested by comparing calculated and experimental structures and energies. If necessary, the initial parameters are then modified to minimize the errors in the calculated output. A discussion of the types of experimental data and the methods that are used to obtain the initial values for metal-dependent parameters is presented below.

(a) Bond stretching and bond angle bending interactions

MM models that use the VFF or POS method require the definition of parameters for metal-dependent bond stretching and angle bending interactions. The VFF method uses parameters for M—L stretches, M—L—X bends, and L—M—L bends. The POS method uses parameters for M—L stretches and M—L—X bends. Both the stretching and the bending deformations are usually described with harmonic potential functions (eqns. (2) and (5)). The parameters needed for M—L bond stretching deformations are the strain-free length, r_0, and the force constant, K_r. The parameters needed for M—L—X and L—M—L bending deformations are the strain-free angle, θ_0, and the bending force constant, K_θ.

The standard approach that has been used to obtain these parameters is a three-step process. First, the force constants, K_r and K_θ, are assigned. These parameters are typically derived from vibrational data. Next, an initial set of strain-free geometric parameters are assigned. Values for r_0 are assigned by comparison with experimental bond lengths in complexes that are deemed to be relatively unstrained. Values for θ_0 are set to correspond to ideal geometries, e.g. $\theta_0 = 90°$ for the *cis*-L—M—L angles in an octahedral geometry. Finally, the geometric parameters are adjusted to give the best agreement between calculated and experimental results. In practice, it is the value of r_0 that is most frequently altered.

The parameters K_r and K_θ are often assigned values of the spectroscopic force constants that are obtained from a normal coordinate analysis of vibrational data. Some care is required when making such assignments. Spectroscopic force constants are obtained by fitting a set of potential functions to vibrational frequencies. The set of potential functions that are used for this purpose differ from those used in MM force fields. As a consequence of this, the force constants that appear in both types of force fields, i.e. K_r and K_θ, can have different numerical values [4,6]. It has been observed that, while the values for K_r are usually either similar or identical within the two types of force field, spectroscopic values for K_θ tend to be 20 to 50% too high for use in MM models [4].

This point has frequently been overlooked in the parameterization of force fields for coordination compounds. Many calculations have been performed with the use of spectroscopic bending force constants. This practice does not cause problems with structures where the bond angles are close to their strain-free values, but it is expected to result in the over-estimation of angle strain in structures where significant deviations from ideal geometries occur. In several cases, it has been reported that better agreement between calculated and experimental results is obtained when spectroscopic bending force constants for L—M—L and M—L—X bending deformations are reduced to half of their value [9,118,138].

With the development of basis sets for metal ions, quantum mechanical calculations offer another means of obtaining stretching and bending force constants [108]. As with the use of spectroscopic data, care must be taken when deriving K_r and K_θ from quantum mechanically derived vibrational frequencies. These frequencies are determined from the increase in potential energy for small displacements from the minimum energy geometry. In MM models, the increase in potential energy that accompanies such displacements is calculated as the sum of many components. It is necessary to factor out the potential energy contributions from other components, e.g. van der Waals and torsional interactions, before values of K_r and K_θ that are appropriate for use in MM calculations can be obtained from the results of quantum mechanical calculations. Two methods for performing this operation have recently been reported [166,167].

In the absence of vibrational data, it is possible to estimate initial values for K_r and K_θ by comparison with values that have been used in other studies. Force fields typically use K_r values in the range of 3–6 mdyn Å^{-1} for the bond stretching of the single bonds found in organic molecules. Without exception, the K_r values that have been assigned to M—L stretching interactions have been below this range. Values in the range of 0.5–2.0 mdyn Å^{-1} have been used in cases where M = Fe, Co, Ni, Cu, Zn, Rh, Pd, Cd, or Pt and L = O, N, S, or P. Empirical relationships between bond lengths and stretching force constants indicate that longer M—L bonds will, in general, have lower force constants [168]. It has been found that K_r values in the range of 0.05–0.20 mdyn Å^{-1} have been required for cases where M = K or La and L = O or N.

Force fields typically use K_θ values in the range of 0.2–1.0 mdyn · Å rad^{-2} for the bending deformations about organic atom centers. The K_θ values that have been assigned to M—L—X bending interactions also fall within this range. Some groups have assumed that the M—L—X bending interaction has the same K_θ value as the analogous C(sp^3)—L—X bending interaction. Other groups use a K_θ value for M—L—X bends that is 1/4 to 1/2 that of the analogous C(sp^3)—L—X value. The values of K_θ that are assigned to L—M—L bends range from 0.3 to 0.7 mdyn · Å rad^{-2}.

(b) Torsional interactions

MM models that use the VFF or POS method require the definition of parameters for M—L—X—X torsional interactions. Torsional interactions are usually described with a Fourier series expansion of the torsional angle (eqn. (8)). The parameters needed for the torsional interactions are the effective barriers to rotation, V_n.

These are among the last parameters to be added to a force field. In organic force fields, they are usually obtained by a trial-and-error fitting process. The values of V_n are adjusted until experimental rotational barriers are reproduced. This operation should be performed only after the van der Waals and electrostatic parameters have been assigned as the non-bonded terms contribute to the calculated rotational barrier. This approach has worked well with organic molecules where there is a large body of data on the height and shape of the rotational barriers for many types of bond.

Much less information is available for rotational barriers of bonds in metal complexes. Therefore, it is usually necessary to guess a value of the effective barriers to rotation for M−L−X−X torsional interactions. One approach that has often been used is to assume that an M−L−X−X interaction will contribute the same amount to a rotational barrier as the corresponding C(sp^3)−L−X−X interaction.

(c) Non-bonded interactions

MM models that employ the ionic method require the definition of van der Waals and electrostatic interaction parameters for the metal ion. The form of the parameters will depend upon the potential functions that are used. For the van der Waals interactions, some codes require the assignment of A and C (eqn. (13)) or A, B, and C (eqn. (14)) for each type of M··X pair. Other codes merely require the definition of r^* and ε for the metal ion (eqns. (15) and (16)).

Various methods have been used to obtain van der Waals parameters for interactions with metal ions. For the alkali metals, van der Waals parameters have been estimated by assuming that they have the same values as the noble gas with the same configuration as each metal ion [157], by adjusting them to yield the best agreement between calculated and experimental binding energies and M−L bond lengths [145], and by fitting to the results of ab initio calculations [154]. For transition metals, van der Waals parameters have been roughly estimated by comparison with values that are used for the elements found in organic compounds [60,62,63,78–82,84–89,98,102,104,106,140].

All MM calculations based on the ionic method have used Coulomb's law to model the electrostatic interactions (eqn. (17)). This approach requires the definition of point charges throughout the complex. Typically, a full formal charge is assigned to the metal ion. The distribution of point charges on the ligand atoms is obtained from quantum mechanical calculations. The procedures to extract the point charge distributions from quantum mechanical calculations continue to evolve [169–172]. Note that, when point charges are added to an organic force field that was developed without them, the values of other parameters in the force field will need to be readjusted. This is particularly true of the parameters that are used for van der Waals and torsional interactions.

MM models that are based upon the VFF and POS methods do not require the addition of non-bonded interactions with the metal ion. The majority of VFF and POS calculations have yielded satisfactory results without including these terms. Where metal ion non-bonded terms have been added [60,62,63,78–82,84–89,98,102,104,106,140], justification for the addition has not been provided. It remains to be shown that the addition of metal ion non-bonded terms to a VFF or POS force field actually improves the performance of the model.

C. COMPILATION OF REPORTED CALCULATIONS ON METAL COMPLEXES

In this final section of the review, the MM calculations that have been reported on coordination compounds are compiled in a format that should be of value to

TABLE 1

Metal complexes for which molecular mechanics calculations have been reported

Each entry consists of an abbreviated formula for a complex, the number of structures for which calculations are reported, the extent to which parameters are reported, the type of force field that was applied to the metal center, the software that was used for the calculation, and the literature citation. Abbreviations for ligands are defined in Scheme 1.

Complex	No. of structures	Report parameters[a]	Force field software[b]	Ref.
$[Li(MeOH)_4]^+$	1	P	C, 12	148
$[Li(12C4)]^+$	1	N	C, 1	67
$[Li(14C4)]^+$	1	N	C, 1	67
$[Li(18C6)]^+$	1	N	C, 16	153
$[Li(B_2 18C6)]^+$	1	P	C, 12	148
$[Li(B_2 18C6)(MeOH)_2]^+$	1	P	C, 12	148
$[Li(B_2 30C10)(MeOH)]^+$	1	P	C, 12	148
$[Li(spherand\text{-}1)]^+$	1	P	C, 12	147
$[Li(spherand\text{-}2)]^+$	1	P	C, 12	147
$[Li(spherand\text{-}3)]^+$	2	P	C, 12	147
$[Li(spherand\text{-}4)]^+$	1	N	C, 12	149
$[Li(lac\text{-}1)]^+$	1	P	C, n.a.	156
$[Li(lac\text{-}2)]^+$	2	P	C, n.a.	156
$[Li(lac\text{-}3)]^+$	2	P	C, n.a.	156
$[Li(lac\text{-}4)]^+$	2	P	C, n.a.	156
$[Li(lac\text{-}5)]^+$	2	P	C, n.a.	156
$[Li(lac\text{-}6)]^+$	1	P	C, n.a.	156
$[Li(enniatinB)]^+$	3	P	C, n.a.	157
$[Na(OH_2)_6]^+$	1	C	C, 12	145
$[NaMeOH)_4]^+$	1	P	C, 12	148
$[Na(pentaglyme)]^+$	1	C	C, 12	145
$[Na(12C4)]^+$	1	N	C, 1	67
$[Na(14C4)]^+$	1	N	C, 1	67
$[Na(18C6)]^+$	6	C	C, 12	145
$[Na(18C6)]^+$	2	N	C, 16	153
$[Na(18C6)(OH_2)]^+$	1	N	C, 17	155
$[Na(18C6)(OH_2)_2]^+$	2	C	C, 12	145
$[Na(B_2 18C6)]^+$	1	P	C, 12	148
$[Na(B_2 18C6)(MeOH)_2]^+$	1	P	C, 12	148
$[Na(B_2 30C10)]^+$	1	P	C, 12	148
$[Na(2,2,2\text{-}crypt)]^+$	6	C	C, 12	146
$[Na(spherand\text{-}1)]^+$	1	P	C, 12	147
$[Na(spherand\text{-}2)]^+$	1	P	C, 12	147
$[Na(spherand\text{-}3)]^+$	2	P	C, 12	147
$[Na(spherand\text{-}4)]^+$	1	N	C, 12	149
$[Na(lac\text{-}1)]^+$	1	P	C, n.a.	156
$[Na(lac\text{-}2)]^+$	2	P	C, n.a.	156
$[Na(lac\text{-}3)]^+$	2	P	C, n.a.	156

TABLE 1 (*continued*)

Complex	No. of structures	Report parameters[a]	Force field software[b]	Ref.
$[\mathrm{Na(lac\text{-}4)}]^{+}$	2	P	C, n.a.	156
$[\mathrm{Na(lac\text{-}6)}]^{+}$	1	P	C, n.a.	156
$[\mathrm{Na(enniatinB)}]^{+}$	6	P	C, n.a.	157
$[\mathrm{Na(enniatinB)_2}]^{+}$	2	P	C, n.a.	157
$[\mathrm{Na(valinomycin)}]^{+}$	1	N	C, n.a.	158
$[\mathrm{Mg(18C6)(dbp)_2(OH_2)}]^{0}$	1	N	C, 18	152
$[\mathrm{K(OH_2)_6}]^{+}$	1	C	C, 12	145
$[\mathrm{K(MeOH)_6}]^{+}$	1	P	C, 12	148
$[\mathrm{K(pentaglyme)}]^{+}$	1	C	C, 12	145
$[\mathrm{K(12C4)}]^{+}$	1	N	C, 1	67
$[\mathrm{K(14C4)}]^{+}$	1	N	C, 1	67
$[\mathrm{K(18C6)}]^{+}$	6	C	C, 12	145
$[\mathrm{K(18C6)}]^{+}$	1	N	C, 16	153
$[\mathrm{K(18C6)}]^{+}$	1	N	C, 16	154
$[\mathrm{K(18C6)(OH_2)_2}]^{+}$	2	C	C, 12	145
$[\mathrm{K(18C6)(OH_2)_2}]^{+}$	1	N	C, 17	155
$[\mathrm{K(B_2 18C6)}]^{+}$	1	P	C, 12	148
$[\mathrm{K(B_2 18C6)(MeOH)_2}]^{+}$	1	P	C, 12	148
$[\mathrm{K(B_2 30C10)}]^{+}$	1	P	C, 12	148
$[\mathrm{K(lac\text{-}1)}]^{+}$	1	P	C, n.a.	156
$[\mathrm{K(lac\text{-}2)}]^{+}$	1	P	C, n.a.	156
$[\mathrm{K(lac\text{-}3)}]^{+}$	2	P	C, n.a.	156
$[\mathrm{K(lac\text{-}6)}]^{+}$	1	P	C, n.a.	156
$[\mathrm{K(18aneN_2O_4\text{-}1)}]^{+}$	1	P	A&C, 7	150
$[\mathrm{K(18aneN_2O_4\text{-}2)}]^{+}$	1	P	A&C, 7	150
$[\mathrm{K(18aneN_2O_4\text{-}3)}]^{+}$	1	P	A&C, 7	150
$[\mathrm{K(2,2,2\text{-}crypt)}]^{+}$	6	C	C, 12	146
$[\mathrm{K(spherand\text{-}1)}]^{+}$	1	P	C, 12	147
$[\mathrm{K(spherand\text{-}2)}]^{+}$	1	P	C, 12	147
$[\mathrm{K(spherand\text{-}4)}]^{+}$	1	N	C, 12	149
$[\mathrm{K(enniatinB)}]^{+}$	6	P	C, n.a.	157
$[\mathrm{K(enniatinB)_2}]^{+}$	2	P	C, n.a.	157
$[\mathrm{K(valinomycin)}]^{+}$	1	N	C, n.a.	158
$[\mathrm{Ca(18C6)(dbp)_2(OH_2)}]^{0}$	1	N	C, 18	152
$[\mathrm{Ca(trispep\text{-}1)}]^{2+}$	1	N	C, n.a.	161
$[\mathrm{Ca(trispep\text{-}2)}]^{2+}$	1	N	C, n.a.	161
$[\mathrm{Ca(trispep\text{-}3)}]^{2+}$	1	N	C, n.a.	161
$[\mathrm{Ca(trispep\text{-}4)}]^{2+}$	1	N	C, n.a.	161
$[\mathrm{Ca(trispep\text{-}5)}]^{2+}$	1	N	C, n.a.	161
$[\mathrm{Ca(trispep\text{-}6)}]^{2+}$	1	N	C, n.a.	161

TABLE 1 (*continued*)

Complex	No. of structures	Report parameters[a]	Force field software[b]	Ref.
$[\text{Cr}^{0}(\text{CO})_{5}]^{0}$	1	P	A, 11	102
$[\text{Cr}^{0}(\text{CO})_{5}]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{PMe}_{3})]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{PMe}_{2}\text{Et})]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{PMeEt}_{2})]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{PEt}_{3})]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{P}(n\text{-Bu})_{3})]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{PMe}_{2}(\text{i-Pr}))]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{PMe}_{2}(t\text{-Bu}))]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{PEt}_{2}(\text{i-Pr}))]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{P}(\text{i-Bu})_{3})]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{PMe}(\text{i-Pr})_{2})]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{PEt}_{2}(t\text{-Bu}))]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{PEt}(\text{i-Pr})_{2})]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{P}(\text{i-Pr})_{3})]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{PMe}(t\text{-Bu})_{2})]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{P}(t\text{-Bu})(\text{i-Pr})_{2})]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{PCy}_{3})]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{P}(\text{i-Pr})(t\text{-Bu})_{2})]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{P}(t\text{-Bu})_{3})]^{0}$	1	P	A, 11	103
$[\text{Cr}^{0}(\text{CO})_{5}(\text{P}(\text{OMe})_{3})]^{0}$	1	P	A, 11	102
$[\text{Cr}^{0}(\text{CO})_{5}(\text{P}(\text{OEt})_{3})]^{0}$	1	P	A, 11	102
$[\text{Cr}^{0}(\text{CO})_{5}(\text{P}(\text{OPh})_{3})]^{0}$	1	P	A, 11	102
$[\text{Cr}^{0}(\text{CO})_{5}(\text{P}(\text{O}i\text{-Pr})_{3})]^{0}$	1	P	A, 11	102
$[\text{Cr}^{0}(\text{CO})_{5}(\text{P}(\text{OCH}_{2})_{3}\text{CMe})]^{0}$	1	P	A, 11	102
$[\text{Cr}^{0}(\text{CO})_{5}(\text{P}(\text{O}t\text{-Bu})_{3})]^{0}$	1	P	A, 11	102
$[\text{Cr}^{0}(\text{CO})_{5}(\text{P}(\text{O}i\text{-Pr})_{2}(\text{O}t\text{-Bu}))]^{0}$	1	P	A, 11	102
$[\text{Cr}^{0}(\text{CO})_{5}(\text{P}(\text{O}i\text{-Pr})(\text{O}t\text{-Bu})_{2})]^{0}$	1	P	A, 11	102
$[\text{Fe}^{\text{III}}(\text{enterobactin})]^{3-}$	2	P	C, n.a.	159
$[\text{Fe}^{\text{III}}(\text{mecam})]^{3-}$	1	P	C, n.a.	159
$[\text{Fe}^{\text{II}}(\text{porphyrin-1})]^{0}$	1	P	A, 7	65
$[\text{Fe}^{\text{II}}(\text{porphyrin-2})(\text{imd})(\text{O}_{2})]^{0}$	1	P	A, 7	65
$[\text{Fe}^{\text{II}}(\text{porphyrin-2})(\text{imd})(\text{CO})]^{0}$	1	P	A, 7	65
$[\text{Co}^{\text{III}}(\text{NH}_{3})_{6}]^{3+}$	1	N	A, 1	53
$[\text{Co}^{\text{III}}(\text{NH}_{3})_{6}]^{3+}$	1	N	B, 2	131
$[\text{Co}^{\text{III}}(\text{NH}_{3})_{6}]^{3+}$	1	P	A, 3	92
$[\text{Co}^{\text{III}}(\text{MeNH}_{2})_{5}(\text{Cl})]^{3+}$	1	N	A, 1	53
$[\text{Co}^{\text{III}}(\text{en})(\text{Cl})_{4}]^{-}$	1	C	A, 4	19
$[\text{Co}^{\text{III}}(\text{en})(\text{NH}_{3})_{4}]^{3+}$	1	P	A, 3	92
$[\text{Co}^{\text{III}}(\text{en})_{2}(\text{NH}_{3})_{2}]^{3+}$	2	P	A, 3	92
$[\text{Co}^{\text{III}}(\text{en})_{2}(N\text{-Me-alaO})]^{2+}$	4	N	A, 1	24
$[\text{Co}^{\text{III}}(\text{en})_{2}(N\text{-Me-glyO})]^{2+}$	2	N	A, 1	24

TABLE 1 (*continued*)

Complex	No. of structures	Report parameters[a]	Force field software[b]	Ref.
$[\mathrm{Co^{III}(en)_3}]^{3+}$	2	N	A, 1	14
$[\mathrm{Co^{III}(en)_3}]^{3+}$	4	N	A, 5	74
$[\mathrm{Co^{III}(en)_3}]^{3+}$	1	N	A, 3	83
$[\mathrm{Co^{III}(en)_3}]^{3+}$	1	P	A, 1	49
$[\mathrm{Co^{III}(en)_3}]^{3+}$	1	N	A, 1	53
$[\mathrm{Co^{III}(en)_3}]^{3+}$	1	N	B, 2	131
$[\mathrm{Co^{III}(en)_3}]^{3+}$	1	P	A, 3	92
$[\mathrm{Co^{III}(en)_2(pn)}]^{3+}$	4	N	A, 1	14
$[\mathrm{Co^{III}(en)(pn)_2}]^{3+}$	2	N	A, 1	14
$[\mathrm{Co^{III}(pn)(Cl)_4}]^{-}$	2	C	A, 4	19
$[\mathrm{Co^{III}(pn)(NH_3)_4}]^{3+}$	2	N	B, 1	119
$[\mathrm{Co^{III}(pn)_3}]^{3+}$	12	C	A, 5	75
$[\mathrm{Co^{III}(pn)_3}]^{3+}$	12	N	B, 1	129
$[\mathrm{Co^{III}}(N\text{-Me-en})(\mathrm{Cl})_4]^{-}$	2	C	A, 4	19
$[\mathrm{Co^{III}}(N,N'\text{-Me}_2\text{-en})(\mathrm{Cl})_4]^{-}$	3	C	A, 4	19
$[\mathrm{Co^{III}}(N_1\text{-Me-pn})(\mathrm{Cl})_4]^{-}$	4	C	A, 4	19
$[\mathrm{Co^{III}}(N_2\text{-Me-pn})(\mathrm{Cl})_4]^{-}$	4	C	A, 4	19
$[\mathrm{Co^{III}(bn)(Cl)_4}]^{-}$	3	C	A, 4	19
$[\mathrm{Co^{III}(bn)(en)_2}]^{3+}$	32	N	A, 5	74
$[\mathrm{Co^{III}(bn)_3}]^{3+}$	8	N	A, 6	70
$[\mathrm{Co^{III}(bn)_3}]^{3+}$	32	C	A, 5	72
$[\mathrm{Co^{III}(bn)_3}]^{3+}$	14	N	A, 5	74
$[\mathrm{Co^{III}(bn)_3}]^{3+}$	16	N	A, 1	41
$[\mathrm{Co^{III}(ibn)_3}]^{3+}$	12	N	A, 5	73
$[\mathrm{Co^{III}(dmbn)(NH_3)_4}]^{3+}$	2	N	B, 1	119
$[\mathrm{Co^{III}(chxn)_3}]^{3+}$	4	C	A, 5	75
$[\mathrm{Co^{III}(pip)(NH_3)_4}]^{3+}$	1	P	A, 3	92
$[\mathrm{Co^{III}(pip)_2(NH_3)_2}]^{3+}$	2	P	A, 3	92
$[\mathrm{Co^{III}(pip)_3}]^{3+}$	1	P	A, 3	92
$[\mathrm{Co^{III}(tn)(Cl)_4}]^{-}$	2	C	A, 4	19
$[\mathrm{Co^{III}(tn)(en)_2}]^{3+}$	10	N	A, 5	77
$[\mathrm{Co^{III}(tn)_2(CO_3)}]^{+}$	3	P	A, 1	12
$[\mathrm{Co^{III}(tn)_2(CO_3)}]^{+}$	1	N	A, 1	53
$[\mathrm{Co^{III}(tn)_2(CO_3)}]^{+}$	1	N	A, 1	18
$[\mathrm{Co^{III}(tn)_2(en)}]^{3+}$	20	N	A, 5	77
$[\mathrm{Co^{III}(tn)_3}]^{3+}$	3	P	A, 1	12
$[\mathrm{Co^{III}(tn)_3}]^{3+}$	16	C	A&B, 6	69
$[\mathrm{Co^{III}(tn)_3}]^{3+}$	16	C	A&B, 6	69
$[\mathrm{Co^{III}(tn)_3}]^{3+}$	18	N	A, 5	71
$[\mathrm{Co^{III}(tn)_3}]^{3+}$	16	N	A, 5	77
$[\mathrm{Co^{III}(tn)_3}]^{3+}$	1	N	A, 1	53
$[\mathrm{Co^{III}(tn)_3}]^{3+}$	1	N	B, 2	131
$[\mathrm{Co^{III}(tn)_3}]^{3+}$	1	P	A, 3	92
$[\mathrm{Co^{III}(1,3\text{-bn})(Cl)_4}]^{-}$	4	C	A, 4	19
$[\mathrm{Co^{III}}(N\text{-Me-tn})(\mathrm{Cl})_4]^{-}$	4	C	A, 4	19

TABLE 1 (*continued*)

Complex	No. of structures	Report parameters[a]	Force field software[b]	Ref.
$[Co^{III}(ptn)(NH_3)_4]^{3+}$	2	P	B, 1	118
$[Co^{III}(ptn)_3]^{3+}$	2	C	A&B, 6	69
$[Co^{III}(ptn)_3]^{3+}$	5	N	A, 6	70
$[Co^{III}(ptn)_3]^{3+}$	10	N	A, 5	71
$[Co^{III}(ptn)_3]^{3+}$	2	N	A, 5	77
$[Co^{III}(mptn)(NH_3)_4]^{3+}$	2	N	B, 1	120
$[Co^{III}(mptn)(CN)_4]^{-}$	2	N	B, 1	120
$[Co^{III}(tmd)_3]^{3+}$	1	P	A, 3	92
$[Co^{III}(dien)(NH_3)_3]^{3+}$	2	N	A, 1	61
$[Co^{III}(dien)(NH_3)_3]^{3+}$	2	P	A, 3	92
$[Co^{III}(dien)(en)(NH_3)]^{3+}$	4	N	A, 1	61
$[Co^{III}(dien)(en)(NH_3)]^{3+}$	4	P	A, 3	92
$[Co^{III}(dien)_2]^{3+}$	3	N	A, 1	15
$[Co^{III}(dien)_2]^{3+}$	1	N	A, 1	18
$[Co^{III}(dien)_2]^{3+}$	4	N	A, 1	27
$[Co^{III}(dien)_2]^{3+}$	3	N	A, 1	29
$[Co^{III}(dien)_2]^{3+}$	18	P	B, 1	125
$[Co^{III}(dien)_2]^{3+}$	1	N	B, 2	131
$[Co^{III}(dien)_2]^{3+}$	4	P	A, 3	92
$[Co^{III}(dien)(dema)]^{3+}$	3	N	A, 1	29
$[Co^{III}(1,2,3\text{-}pn)_2]^{3+}$	1	N	A, 1	53
$[Co^{III}(1,2,3\text{-}pn)_2]^{3+}$	1	N	B, 2	131
$[Co^{III}(1,2,3\text{-}pn)_2]^{3+}$	2	N	B, 2	132
$[Co^{III}(trab)_2]^{3+}$	16	N	B, 2	134
$[Co^{III}(dpt)(en)(Cl)]^{2+}$	7	N	A, 1	13
$[Co^{III}(dpt)(dien)]^{3+}$	15	N	B, 1	122
$[Co^{III}(dpt)(dien)]^{3+}$	1	N	B, 1	123
$[Co^{III}(dpt)_2]^{3+}$	30	N	B, 1	121
$[Co^{III}(dpt)_2]^{3+}$	1	N	B, 2	131
$[Co^{III}(dpt)_2]^{3+}$	3	P	A, 3	92
$[Co^{III}(trien)(en)]^{3+}$	3	N	A, 1	61
$[Co^{III}(trien)(en)]^{3+}$	3	P	A, 3	92
$[Co^{III}(trien)(NH_3)_2]^{3+}$	2	N	A, 1	42
$[Co^{III}(trien)(NH_3)_2]^{3+}$	5	N	A, 1	57
$[Co^{III}(trien)(NH_3)_2]^{3+}$	5	P	A, 3	92
$[Co^{III}(trien)(Cl)_2]^{+}$	1	N	B, 1	126
$[Co^{III}(trien)(glyO)]^{2+}$	2	N	A, 1	14
$[Co^{III}(trien)(glyO)]^{2+}$	2	C	A, 1	23
$[Co^{III}(trien)(glyO)]^{2+}$	5	N	A, 1	26
$[Co^{III}(trien)(N\text{-}Me\text{-}glyO)]^{2+}$	3	N	A, 1	14
$[Co^{III}(trien)(N\text{-}Me\text{-}glyO)]^{2+}$	4	N	A, 1	24
$[Co^{III}(trien)(N\text{-}Me\text{-}alaO)]^{2+}$	4	N	A, 1	11
$[Co^{III}(trien)(N\text{-}Me\text{-}alaO)]^{2+}$	4	N	A, 1	24
$[Co^{III}(trien)(proO)]^{2+}$	4	C	A, 1	10
$[Co^{III}(trien)(proO)]^{2+}$	4	N	A, 1	14

TABLE 1 (*continued*)

Complex	No. of structures	Report parameters[a]	Force field software[b]	Ref.
$[\mathrm{Co^{III}}(2,2,3\text{-tet})(\mathrm{Cl})_2]^{+}$	6	N	A, 1	36
$[\mathrm{Co^{III}}(2,2,3\text{-tet})(\mathrm{Cl})_2]^{+}$	2	N	B, 1	126
$[\mathrm{Co^{III}}(2,10\text{-}\mathrm{Me_2}\text{-}2,3,2\text{-tet})(\mathrm{alaO})]^{2+}$	4	N	A, 1	39
$[\mathrm{Co^{III}}(2,10\text{-}\mathrm{Me_2}\text{-}2,3,2\text{-tet})(N\text{-}\mathrm{Me\text{-}alaO})]^{2+}$	2	N	A, 1	40
$[\mathrm{Co^{III}}(5\text{-}\mathrm{Me}\text{-}3,2,3\text{-tet})(\mathrm{Cl})_2]^{+}$	9	N	A, 4	20
$[\mathrm{Co^{III}}(3,10\text{-}\mathrm{Me_2}\text{-}3,2,3\text{-tet})(\mathrm{Cl})_2]^{+}$	6	N	A, 1	50
$[\mathrm{Co^{III}}(\mathrm{tetraen})(\mathrm{Cl})]^{2+}$	1	C	A, 1	9
$[\mathrm{Co^{III}}(\mathrm{tetraen})(\mathrm{Cl})]^{2+}$	2	N	A, 1	16
$[\mathrm{Co^{III}}(\mathrm{tetraen})(\mathrm{NH_3})]^{3+}$	8	N	A, 1	61
$[\mathrm{Co^{III}}(\mathrm{tetraen})(\mathrm{NH_3})]^{3+}$	8	P	A, 3	92
$[\mathrm{Co^{III}}(\mathrm{pyht})(\mathrm{alaO})]^{2+}$	2	N	A, 1	39
$[\mathrm{Co^{III}}(\mathrm{picpn})(\mathrm{glyO})]^{2+}$	2	N	A, 1	22
$[\mathrm{Co^{III}}(\mathrm{picpn})(\mathrm{alaO})]^{2+}$	4	N	A, 1	22
$[\mathrm{Co^{III}}(\mathrm{picpn})(\mathrm{ox})]^{+}$	6	N	A, 1	17
$[\mathrm{Co^{III}}(\mathrm{tren})(\mathrm{NH_3})(\mathrm{Cl})]^{2+}$	2	C	A, 1	25
$[\mathrm{Co^{III}}(\mathrm{tren})(\mathrm{glyO})]^{2+}$	2	N	A, 1	28
$[\mathrm{Co^{III}}(\mathrm{Me\text{-}tren})(\mathrm{NH_3})(\mathrm{Cl})]^{2+}$	6	N	A, 1	47
$[\mathrm{Co^{III}}(\mathrm{pentaen})]^{3+}$	8	N	A, 1	27
$[\mathrm{Co^{III}}(\mathrm{pentaen})]^{3+}$	8	P	A, 3	92
$[\mathrm{Co^{III}}(\mathrm{edta})]^{-}$	1	P	A, 1	32
$[\mathrm{Co^{III}}(\mathrm{edds})]^{-}$	1	N	A, 1	33
$[\mathrm{Co^{III}}(\mathrm{dbta})]^{-}$	3	N	A, 1	48
$[\mathrm{Co^{III}}(\mathrm{Me_2\text{-}sal_2tn})(\mathrm{sal})]^{0}$	9	N	A, 3	91
$[\mathrm{Co^{III}}(\mathrm{daes})_2]^{3+}$	16	C	A, 5	75
$[\mathrm{Co^{III}}(\mathrm{aeaps})_2]^{3+}$	8	C	A, 5	75
$[\mathrm{Co^{III}}(9\mathrm{aneN_3})_2]^{3+}$	1	N	A, 1	53
$[\mathrm{Co^{III}}(9\mathrm{aneN_3})_2]^{3+}$	1	N	B, 2	131
$[\mathrm{Co^{III}}(10\mathrm{aneN_3})_2]^{+}$	16	N	A, 1	46
$[\mathrm{Co^{III}}(12\mathrm{aneN_4})(\mathrm{NO_2})_2]^{+}$	1	N	A, 1	53
$[\mathrm{Co^{III}}(13\mathrm{aneN_4})(\mathrm{Cl})_2]^{+}$	1	N	A, 4	30
$[\mathrm{Co^{III}}(13\mathrm{aneN_4})(\mathrm{Cl})_2]^{+}$	1	N	A, 4	31
$[\mathrm{Co^{III}}(13\mathrm{aneN_4})(\mathrm{Cl})_2]^{+}$	1	N	B, 1	126
$[\mathrm{Co^{III}}(14\mathrm{aneN_4})(\mathrm{Cl})_2]^{+}$	1	N	A, 4	30
$[\mathrm{Co^{III}}(14\mathrm{aneN_4})(\mathrm{Cl})_2]^{+}$	1	N	A, 4	31
$[\mathrm{Co^{III}}(14\mathrm{aneN_4})(\mathrm{Cl})_2]^{+}$	1	N	B, 1	126
$[\mathrm{Co^{III}}(14\mathrm{aneN_4})(\mathrm{Me})(\mathrm{OH_2})]^{2+}$	1	N	A, 3	94
$[\mathrm{Co^{III}}(14\mathrm{aneN_4})(\mathrm{Me})]^{2+}$	1	N	A, 3	94
$[\mathrm{Co^{III}}(\mathrm{diammac})]^{3+}$	1	N	B, 2	131
$[\mathrm{Co^{III}}(\mathrm{Me_6\text{-}14dieneN_4\text{-}1})(\mathrm{Cl})_2]^{+}$	2	N	A, 3	93
$[\mathrm{Co^{III}}(\mathrm{Me_6\text{-}14dieneN_4\text{-}1})(\mathrm{Cl})]^{2+}$	5	N	A, 3	93
$[\mathrm{Co^{III}}(\mathrm{Me_6\text{-}14dieneN_4\text{-}1})(\mathrm{Cl})(\mathrm{OH_2})]^{+}$	3	N	A, 3	93
$[\mathrm{Co^{III}}(\mathrm{Me_6\text{-}14dieneN_4\text{-}1})(\mathrm{OH_2})]^{2+}$	3	N	A, 3	93
$[\mathrm{Co^{III}}(\mathrm{Me_6\text{-}14dieneN_4\text{-}1})(\mathrm{Cl})(\mathrm{Me})]^{+}$	3	N	A, 3	93
$[\mathrm{Co^{III}}(\mathrm{Me_6\text{-}14dieneN_4\text{-}1})(\mathrm{OH_2})(\mathrm{Me})]^{+}$	3	N	A, 3	94
$[\mathrm{Co^{III}}(\mathrm{Me_6\text{-}14dieneN_4\text{-}1})(\mathrm{Me})]^{2+}$	3	N	A, 3	93

TABLE 1 (*continued*)

Complex	No. of structures	Report parameters[a]	Force field software[b]	Ref.
$[\mathrm{Co^{III}(Me_6\text{-}14dieneN_4\text{-}1)(Me)}]^{2+}$	3	N	A, 3	94
$[\mathrm{Co^{III}(Me_4\text{-}14tetraeneN_4)(OH_2)(Me)}]^{+}$	1	N	A, 3	94
$[\mathrm{Co^{III}(Me_4\text{-}14tetraeneN_4)(Me)}]^{2+}$	1	N	A, 3	94
$[\mathrm{Co^{III}(15aneN_4\text{-}1)(Cl)_2}]^{+}$	2	N	A, 4	30
$[\mathrm{Co^{III}(15aneN_4\text{-}1)(Cl)_2}]^{+}$	2	N	A, 4	31
$[\mathrm{Co^{III}(15aneN_4\text{-}1)(Cl)_2}]^{+}$	1	N	B, 1	126
$[\mathrm{Co^{III}(Me(NH_2)(1,4\text{-}C_2)\text{-}15aneN_4)(Cl)_2}]^{+}$	3	N	A, 7	68
$[\mathrm{Co^{III}(16aneN_4)(Cl)_2}]^{+}$	1	N	A, 4	30
$[\mathrm{Co^{III}(16aneN_4)(Cl)_2}]^{+}$	1	N	A, 4	31
$[\mathrm{Co^{III}(16aneN_4)(Cl)_2}]^{+}$	2	N	B, 1	126
$[\mathrm{Co^{III}(18aneN_6)}]^{3+}$	3	N	A, 1	34
$[\mathrm{Co^{III}(18aneN_6)}]^{3+}$	3	P	A, 3	92
$[\mathrm{Co^{III}(20aneN_6)}]^{3+}$	6	N	A, 1	45
$[\mathrm{Co^{III}(sep)}]^{3+}$	4	P	A, 1	49
$[\mathrm{Co^{III}(sep)}]^{3+}$	5	P	B, 1	125
$[\mathrm{Co^{III}(sep)}]^{3+}$	1	N	B, 2	131
$[\mathrm{Co^{III}(azacapten)}]^{3+}$	2	P	B, 1	127
$[\mathrm{Co^{III}(sar)}]^{3+}$	1	N	B, 2	131
$[\mathrm{Co^{III}(sar)}]^{3+}$	6	N	B, 2	133
$[\mathrm{Co^{II}(NH_3)_6}]^{2+}$	1	N	B, 2	131
$[\mathrm{Co^{II}(en)_3}]^{2+}$	1	P	A, 1	49
$[\mathrm{Co^{II}(en)_3}]^{2+}$	1	N	B, 2	131
$[\mathrm{Co^{II}(pn)_3}]^{2+}$	4	N	B, 1	129
$[\mathrm{Co^{II}(tn)_3}]^{2+}$	1	N	B, 2	131
$[\mathrm{Co^{II}(dien)_2}]^{2+}$	13	P	B, 1	125
$[\mathrm{Co^{II}(dien)_2}]^{2+}$	1	N	B, 2	131
$[\mathrm{Co^{II}(dpt)_2}]^{2+}$	1	N	B, 2	131
$[\mathrm{Co^{II}(1,2,3\text{-}pn)_2}]^{2+}$	1	N	B, 2	131
$[\mathrm{Co^{II}(9aneN_3)_2}]^{2+}$	1	N	B, 2	131
$[\mathrm{Co^{II}(diammac)}]^{2+}$	1	N	B, 2	131
$[\mathrm{Co^{II}(sep)}]^{2+}$	4	P	A, 1	49
$[\mathrm{Co^{II}(sep)}]^{2+}$	5	P	B, 1	125
$[\mathrm{Co^{II}(sep)}]^{2+}$	1	N	B, 2	131
$[\mathrm{Co^{II}(azacapten)}]^{2+}$	2	P	B, 1	127
$[\mathrm{Co^{II}(sar)}]^{2+}$	1	N	B, 2	131
$[\mathrm{Ni^{II}(OH_2)_6}]^{2+}$	1	N	A, 1	38
$[\mathrm{Ni^{II}(NH_3)_6}]^{2+}$	1	N	A, 1	53
$[\mathrm{Ni^{II}(NH_3)_6}]^{2+}$	1	P	A, 3	92
$[\mathrm{Ni^{II}(en)(OH_2)_4}]^{2+}$	1	P	A, 1	37
$[\mathrm{Ni^{II}(en)(OH_2)_4}]^{2+}$	1	N	A, 1	38
$[\mathrm{Ni^{II}(en)(NH_3)_4}]^{2+}$	1	P	A, 3	92
$[\mathrm{Ni^{II}(en)_2(OH_2)_2}]^{2+}$	1	P	A, 1	37

TABLE 1 (*continued*)

Complex	No. of structures	Report parameters[a]	Force field software[b]	Ref.
$[Ni^{II}(en)_2(OH_2)_2]^{2+}$	1	N	A, 1	38
$[Ni^{II}(en)_2]^{2+}$	1	N	A, 1	53
$[Ni^{II}(en)_2]^{2+}$	1	N	A, 7	63
$[Ni^{II}(en)_3]^{2+}$	1	P	A, 1	37
$[Ni^{II}(en)_3]^{2+}$	1	C	A, 1	35
$[Ni^{II}(en)_3]^{2+}$	1	N	A, 1	38
$[Ni^{II}(en)_3]^{2+}$	1	N	A, 1	53
$[Ni^{II}(en)_3]^{2+}$	1	P	A, 3	92
$[Ni^{II}(tn)(OH_2)_4]^{2+}$	1	P	A, 1	37
$[Ni^{II}(tn)_2(OH_2)_2]^{2+}$	1	P	A, 1	37
$[Ni^{II}(tn)_3]^{2+}$	1	P	A, 1	37
$[Ni^{II}(tn)_3]^{2+}$	1	C	A, 1	35
$[Ni^{II}(tn)_3]^{2+}$	1	N	A, 1	53
$[Ni^{II}(daco)_2]^{2+}$	1	N	A, 1	52
$[Ni^{II}(daco)_2]^{2+}$	1	N	A, 1	53
$[Ni^{II}(daco)_2]^{2+}$	1	N	A, 7	63
$[Ni^{II}(dien)(OH_2)_3]^{2+}$	1	P	A, 1	37
$[Ni^{II}(dien)(OH_2)_3]^{2+}$	1	N	A, 1	38
$[Ni^{II}(dien)(NH_3)_3]^{2+}$	2	P	A, 3	92
$[Ni^{II}(dien)_2]^{2+}$	1	P	A, 1	37
$[Ni^{II}(dien)_2]^{2+}$	1	C	A, 1	35
$[Ni^{II}(dien)_2]^{2+}$	1	N	A, 1	38
$[Ni^{II}(dien)_2]^{2+}$	1	N	A, 1	53
$[Ni^{II}(dien)_2]^{2+}$	1	P	A, 3	92
$[Ni^{II}(dpt)(OH_2)_3]^{2+}$	1	P	A, 1	37
$[Ni^{II}(dpt)_2]^{2+}$	1	C	A, 1	35
$[Ni^{II}(dpt)_2]^{2+}$	1	P	A, 1	37
$[Ni^{II}(dpt)_2]^{2+}$	1	N	A, 1	53
$[Ni^{II}(2,3,2\text{-}tet)(OH_2)_2]^{2+}$	1	P	A, 1	37
$[Ni^{II}(trien)(OH_2)_2]^{2+}$	1	P	A, 1	37
$[Ni^{II}(trien)(OH_2)_2]^{2+}$	1	N	A, 1	38
$[Ni^{II}(trien)(NH_3)_2]^{2+}$	2	P	A, 3	92
$[Ni^{II}(2,3,2\text{-}tet)(OH_2)_2]^{2+}$	1	N	A, 1	44
$[Ni^{II}(tetraen)(OH_2)]^{2+}$	1	N	A, 1	38
$[Ni^{II}(pentaen)]^{2+}$	1	N	A, 1	38
$[Ni^{II}(BPAAP\text{-}valO)]^{+}$	3	N	A, 7	59
$[Ni^{II}(NPAAP\text{-}valO)]^{+}$	2	N	A, 7	64
$[Ni^{II}(daes)_2]^{2+}$	1	C	A, 7	62
$[Ni^{II}(9aneN_3)_2]^{2+}$	1	N	A, 1	53
$[Ni^{II}(9aneN_3)_2]^{2+}$	2	C	A, 7	62
$[Ni^{II}(9aneN_2S)_2]^{2+}$	2	C	A, 7	62
$[Ni^{II}(9aneNS_2)_2]^{2+}$	2	C	A, 7	62
$[Ni^{II}(9aneS_3)_2]^{2+}$	2	C	A, 7	62
$[Ni^{II}(9aneN_2O)_2]^{2+}$	1	N	A, 1	54
$[Ni^{II}(1,4\text{-}C_2\text{-}12aneN_4)]^{2+}$	1	N	A, 7	63

TABLE 1 (*continued*)

Complex	No. of structures	Report parameters[a]	Force field software[b]	Ref.
$[\mathrm{Ni^{II}(1,4\text{-}C_2\text{-}12aneN_4)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(13aneN_4)}]^{2+}$	1	N	A, 7	63
$[\mathrm{Ni^{II}(Me_2\text{-}13aneN_4)}]^{2+}$	5	P	A, 8	106
$[\mathrm{Ni^{II}(14aneN_4)}]^{2+}$	5	P	A, 8	106
$[\mathrm{Ni^{II}(14aneN_4)(OH_2)_2}]^{2+}$	1	N	A, 1	44
$[\mathrm{Ni^{II}(isocyclam)}]^{2+}$	1	C	A, 1	51
$[\mathrm{Ni^{II}_2((14aneN_4)_2\text{-}1)}]^{4+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}_2((14aneN_4)_2\text{-}2)}]^{4+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(Me_2\text{-}14aneN_4\text{-}1)}]^{2+}$	1	N	A, 7	63
$[\mathrm{Ni^{II}(Me_2\text{-}14aneN_4\text{-}1)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(Me_2\text{-}14aneN_4\text{-}2)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(Me_4\text{-}14aneN_4\text{-}1)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(Me_4\text{-}14aneN_4\text{-}2)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(Me_6\text{-}14aneN_4)}]^{2+}$	3	P	A, 8	106
$[\mathrm{Ni^{II}(Me_2Et_2\text{-}14aneN_4)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(Me_8\text{-}14aneN_4)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(Me_2Py\text{-}14aneN_4)}]^{2+}$	1	N	A, 3	86
$[\mathrm{Ni^{II}(Me_2Py\text{-}14aneN_4)(NO_2)_2}]^{0}$	3	N	A, 3	86
$[\mathrm{Ni^{II}(Me_2Py\text{-}14aneN_4)(en)}]^{2+}$	1	N	A, 3	86
$[\mathrm{Ni^{II}(chxn\text{-}14aneN_4)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(Me_2DMC)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(TMC)}]^{2+}$	2	N	B, 1	124
$[\mathrm{Ni^{II}(TMC)}]^{2+}$	5	C	B, 2	128
$[\mathrm{Ni^{II}(TMC)}]^{2+}$	10	N	A, 9	99
$[\mathrm{Ni^{II}(TMC)}]^{2+}$	1	N	A, 7	63
$[\mathrm{Ni^{II}(TMC)}]^{2+}$	2	P	A, 8	106
$[\mathrm{Ni^{II}(TMC)(N)}]^{2+}$	2	N	B, 1	124
$[\mathrm{Ni^{II}(TMC)(N)}]^{2+}$	7	C	B, 2	128
$[\mathrm{Ni^{II}(TMC)(N_2)}]^{2+}$	2	N	B, 1	124
$[\mathrm{Ni^{II}(TMC)(N_2)}]^{2+}$	5	C	B, 2	128
$[\mathrm{Ni^{II}(Me_6\text{-}TMC)}]^{2+}$	2	P	A, 8	106
$[\mathrm{Ni^{II}(B_2\text{-}14dieneN_4)}]^{2+}$	5	N	A, 8	105
$[\mathrm{Ni^{II}(B_2\text{-}14dieneN_4)(SCN)_2}]^{0}$	5	N	A, 8	105
$[\mathrm{Ni^{II}(B_2Me\text{-}14dieneN_4)}]^{2+}$	10	N	A, 8	105
$[\mathrm{Ni^{II}(B_2Me\text{-}14dieneN_4)(SCN)_2}]^{0}$	10	N	A, 8	105
$[\mathrm{Ni^{II}(Me_2Py\text{-}14dieneN_4)}]^{2+}$	1	N	A, 3	86
$[\mathrm{Ni^{II}(Me_4\text{-}14dieneN_4\text{-}1)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(Me_4\text{-}14dieneN_4\text{-}2)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(Me_6\text{-}14dieneN_4\text{-}1)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(Me_6\text{-}14dieneN_4\text{-}2)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(Me_8\text{-}14dieneN_4)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(cap,Me\text{-}14aneN_6)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(15aneN_4\text{-}2)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(Me_6\text{-}15dieneN_4)}]^{2+}$	1	P	A, 8	106
$[\mathrm{Ni^{II}(15aneN_2OS_2)(OH_2)}]^{2+}$	1	C	A, 7	62

TABLE 1 (*continued*)

Complex	No. of structures	Report parameters[a]	Force field software[b]	Ref.
$[\mathrm{Ni^{II}(porphyrin\text{-}1)}]^0$	1	P	A, 7	65
$[\mathrm{Ni^{II}(porphyrin\text{-}3)}]^+$	5	P	A, 10	100
$[\mathrm{Ni^{II}(porphyrin\text{-}4)}]^+$	1	P	A, 11	104
$[\mathrm{Ni^{II}(B_2\text{-}17dieneN_3O_2)}]^{2+}$	2	N	n.a.	107
$[\mathrm{Ni^{II}(B_2Me_2\text{-}17dieneN_3O_2)}]^{2+}$	2	N	n.a.	107
$[\mathrm{Cu^{II}(thrO)_2}]^0$	53	C	A, 5	78
$[\mathrm{Cu^{II}(ileuO)_2}]^0$	43	C	A, 5	78
$[\mathrm{Cu^{II}}(N,N\text{-}\mathrm{Me_2\text{-}valO})_2]^0$	42	N	A, 5	79
$[\mathrm{Cu^{II}}(N,N\text{-}\mathrm{Me_2\text{-}valO})_2]^0$	20	P	A, 5	81
$[\mathrm{Cu^{II}}(N,N\text{-}\mathrm{Me_2\text{-}valO})_2]^0$	2	N	A, 5	82
$[\mathrm{Cu^{II}}(N,N\text{-}\mathrm{Me_2\text{-}ileuO})_2]^0$	32	N	A, 5	80
$[\mathrm{Cu^{II}_2(MeCO_2)_4(O)_2}]^{4-}$	1	C	A, 1	60
$[\mathrm{Cu^{II}(N_6O_6podand)}]^{2+}$	2	P	A, 3	85
$[\mathrm{Cu^{II}(daes)_2}]^{2+}$	1	C	A, 7	62
$[\mathrm{Cu^{II}(9aneN_2S)_2}]^{2+}$	1	C	A, 7	62
$[\mathrm{Cu^{II}(12aneS_4)(OH_2)}]^{2+}$	1	N	A, 1	56
$[\mathrm{Cu^{II}(13aneS_4)(OH_2)}]^{2+}$	1	N	A, 1	56
$[\mathrm{Cu^{II}(14aneS_4)(OH_2)_2}]^{2+}$	1	N	A, 1	56
$[\mathrm{Cu^{II}(15aneS_4)(OH_2)_2}]^{2+}$	1	N	A, 1	56
$[\mathrm{Cu^{II}(15aneS_5)}]^{2+}$	1	N	A, 1	56
$[\mathrm{Cu^{II}(16aneS_4)(OH_2)_2}]^{2+}$	1	N	A, 1	56
$[\mathrm{Cu^{II}_2(20tetraeneN_4O_2)(NCMe)_2}]^{4+}$	1	P	A, 3	88
$[\mathrm{Cu^{II}_2(20tetraeneN_4O_2)(SCN)_2}]^0$	13	P	A, 3	88
$[\mathrm{Cu^{II}_2(20tetraeneN_4O_2)(pyz)_2}]^{4+}$	1	P	A, 3	88
$[\mathrm{Cu^{II}_2(20tetraeneN_4O_2)(pyzd)_2}]^{4+}$	1	P	A, 3	88
$[\mathrm{Cu^{II}_2(20tetraeneN_4O_2)(dppm)_2}]^{4+}$	1	P	A, 3	88
$[\mathrm{Cu^{II}_2(Me_4\text{-}20tetraeneN_4O_2)(NCMe)_2}]^{4+}$	1	P	A, 3	88
$[\mathrm{Zn^{II}(imd)_3(OH)}]^+$	1	P	A, 12	98
$[\mathrm{Zn^{II}(imd)_3(OH_2)}]^{2+}$	1	P	A, 12	98
$[\mathrm{Zn^{II}(R\text{-}imd)_3(OH)}]^+$	1	P	A, 12	98
$[\mathrm{Zn^{II}(R\text{-}imd)_3(OH_2)}]^{2+}$	1	P	A, 12	98
$[\mathrm{Zn^{II}(his\text{-}CA)_3(OH_2)}]^{2+}$	1	P	C, 13	151
$[\mathrm{Zn^{II}(his\text{-}CA)_3(OH_2)}]^{2+}$	1	P	C, 13	162
$[\mathrm{Zn^{II}(his\text{-}CA)_3(OH_2)}]^{2+}$	1	P	C, 13	163
$[\mathrm{Zn^{II}(his\text{-}CA)_3(OH_2)_2}]^{2+}$	2	P	C, 13	163
$[\mathrm{Zn^{II}(his\text{-}CA)_3(OH_2)_2}]^{2+}$	1	N	C, 13	164
$[\mathrm{Zn^{II}(his\text{-}CA)_3(OH_2)_2}]^{2+}$	1	P	C, 13	165
$[\mathrm{Zn^{II}(his\text{-}CA)_3(HCO_3^-)}]^+$	1	P	C, 13	151
$[\mathrm{Zn^{II}(his\text{-}CA)_3(HCO_3^-)}]^+$	1	P	C, 13	162
$[\mathrm{Zn^{II}(his\text{-}CA)_3(HCO_3^-)}]^+$	2	P	C, 13	163
$[\mathrm{Zn^{II}(his\text{-}CA)_3(HCO_3^-)}]^+$	4	N	C, 13	164
$[\mathrm{Zn^{II}(his\text{-}CA)_3(HCO_3^-)}]^+$	1	P	C, 13	165
$[\mathrm{Zn^{II}(his\text{-}CA)_3(RSO_2NH_2)}]^{2+}$	2	P	C, 13	151

TABLE 1 (*continued*)

Complex	No. of structures	Report parameters[a]	Force field software[b]	Ref.
$[Zn^{II}(his\text{-}CA)_3(RSO_2NH_2)]^{2+}$	2	P	C, 13	162
$[Zn^{II}(his\text{-}CA)_3(RSO_2NH_2)]^{2+}$	2	P	C, 13	163
$[Zn^{II}(his\text{-}CA)_3(RSO_2NH_2)]^{2+}$	1	N	C, 13	164
$[Zn^{II}(his\text{-}CA)_3(RSO_2NH_2)]^{2+}$	1	P	C, 13	165
$[Zn^{II}(porphyrin\text{-}1)]^0$	1	P	A, 7	65
$[Rb(OH_2)_6]^+$	1	C	C, 12	145
$[Rb(MeOH)_6]^+$	1	P	C, 12	148
$[Rb(pentaglyme)]^+$	1	C	C, 12	145
$[Rb(18C6)(OH_2)_2]^+$	1	C	C, 12	145
$[Rb(18C6)(OH_2)_2]^+$	1	N	C, 17	155
$[Rb(B_2 18C6)]^+$	1	P	C, 12	148
$[Rb(B_2 18C6)(MeOH)_2]^+$	1	P	C, 12	148
$[Rb(B_2 30C10)]^+$	1	P	C, 12	148
$[Rb(2,2,2\text{-}crypt)]^+$	1	C	C, 12	146
$[Rb(spherand\text{-}4)]^+$	1	N	C, 12	149
$[Rb(enniatinB)]^+$	4	P	C, n.a.	157
$[Rb(enniatinB)_2]^+$	2	P	C, n.a.	157
$[Rb(valinomycin)]^+$	1	N	C, n.a.	158
$[Sr(18C6)(dbp)_2(OH_2)]^0$	1	N	C, 18	152
$[Rh^{II}{}_2(MeCO_2)_4(OH_2)_2]^0$	1	C	A, 1	66
$[Rh^{II}{}_2(MeCO_2)_4(Me_2SO)_2]^0$	1	C	A, 1	66
$[Rh^{II}{}_2(EtCO_2)_4(Me_2SO)_2]^0$	1	C	A, 1	66
$[Rh^{II}{}_2(CF_3CO_2)_4(Me_2SO)_2]^0$	1	C	A, 1	66
$[Rh^{II}{}_2(t\text{-}BuCO_2)_4(OH_2)_2]^0$	1	C	A, 1	66
$[Rh^{II}{}_2(MeCO_2)_4(O)_2]^{4-}$	1	C	A, 1	60
$[Rh^{II}{}_2(MeCOS)_4(O)_2]^{4-}$	1	C	A, 1	60
$[Rh^{II}{}_2(MeCS_2)_4(O)_2]^{4-}$	1	C	A, 1	60
$[Rh^{II}{}_2(MeCO_2)_4(S)_2]^{4-}$	1	C	A, 1	60
$[Rh^{II}{}_2(MeCOS)_4(S)_2]^{4-}$	1	C	A, 1	60
$[Rh^{II}{}_2(MeCS_2)_4(S)_2]^{4-}$	1	C	A, 1	60
$[Rh^{II}{}_2(MeCO_2)_4]^0$	1	C	A, 1	60
$[Rh^{II}{}_2(MeCOS)_4]^0$	1	C	A, 1	60
$[Rh^{II}{}_2(MeCS_2)_4]^0$	1	C	A, 1	60
$[Rh^I(PMe_3)_4]^+$	1	P	A, 14	108
$[Rh^I(PMe_2Ph)_4]^+$	1	P	A, 14	108
$[Rh^I(dmpe)_2]^+$	1	P	A, 14	108
$[Rh^I(chphos)_2]^+$	1	P	A, 14	108
$[Rh^I(chphos)(cod)]^+$	1	P	A, 14	108
$[Rh^I(dipamp)(cod)]^+$	1	P	A, 14	108
$[Rh^I(dppb)(cod)]^+$	1	P	A, 14	108
$[Rh^I(dipamp)(nbd)]^+$	1	P	A, 14	108

TABLE 1 (*continued*)

Complex	No. of structures	Report parameters^{a}	Force field software^{b}	Ref.
$[\mathrm{Rh^{I}(bdpbp)(nbd)}]^{+}$	1	P	A, 14	108
$[\mathrm{Rh^{I}(cycphos)(nbd)}]^{+}$	3	P	A, 14	108
$[\mathrm{Rh^{I}(chphos)(aac)}]^{+}$	1	P	A, 14	108
$[\mathrm{Rh^{I}(dipamp)(aaa)}]^{+}$	1	P	A, 14	108
$[\mathrm{Rh^{I}(dppe)(aac)}]^{+}$	1	P	A, 14	108
$[\mathrm{Pd^{II}{}_2(MeCO_2)_4}]^{0}$	1	C	A, 1	60
$[\mathrm{Pd^{II}{}_2(MeCS_2)_4}]^{0}$	1	C	A, 1	60
$[\mathrm{Cd^{II}{}_2(MeCO_2)_4(PPh_3)_2}]^{4-}$	1	C	A, 1	60
$[\mathrm{Cs(OH_2)_6}]^{+}$	1	C	C, 12	145
$[\mathrm{Cs(MeOH)_4}]^{+}$	1	P	C, 12	148
$[\mathrm{Cs(pentaglyme)}]^{+}$	1	C	C, 12	145
$[\mathrm{Cs(18C6)(OH_2)_2}]^{+}$	2	C	C, 12	145
$[\mathrm{Cs(18C6)(OH_2)_2}]^{+}$	1	N	C, 17	155
$[\mathrm{Cs(2,2,2\text{-}crypt)}]^{+}$	1	C	C, 12	146
$[\mathrm{Cs(B_2\,18C6)}]^{+}$	1	P	C, 12	148
$[\mathrm{Cs(B_2\,18C6)(MeOH)_2}]^{+}$	1	P	C, 12	148
$[\mathrm{Cs(B_2\,30C10)}]^{+}$	1	P	C, 12	148
$[\mathrm{Cs(spherand\text{-}4)}]^{+}$	1	N	C, 12	149
$[\mathrm{Cs(enniatinB)}]^{+}$	2	P	C, n.a.	157
$[\mathrm{Cs(enniatinB)_2}]^{+}$	2	P	C, n.a.	157
$[\mathrm{Cs(valinomycin)}]^{+}$	1	N	C, n.a.	158
$[\mathrm{Ba(18C6)(dbp)_2(OH_2)}]^{0}$	1	N	C, 18	152
$[\mathrm{Ba(20tetraeneN_4O_2)(OH_2)_2}]^{2+}$	1	P	A, 3	88
$[\mathrm{Pt^{II}(mptn)(bpy)}]^{2+}$	2	N	B, 1	120
$[\mathrm{Pt^{II}(9Et\text{-}gua)_2(NH_3)_2)}]^{2+}$	2	P	B, 2	136
$[\mathrm{Pt^{II}(9Et\text{-}gua)_2(tmen)}]^{2+}$	2	P	B, 2	136
$[\mathrm{Pt^{II}(guo)_2(NH_3)_2)}]^{2+}$	2	P	B, 2	136
$[\mathrm{Pt^{II}(5'\text{-}gmp)(NH_3)_2)}]^{2+}$	4	N	B, 2	137
$[\mathrm{Pt^{II}(5'\text{-}gtp)(NH_3)_2)}]^{2+}$	7	N	B, 2	137
$[\mathrm{Pt^{II}(9Et\text{-}ade)_2(NH_3)_2)}]^{2+}$	2	P	B, 2	136
$[\mathrm{Pt^{II}(9Et\text{-}ade)_2(en)}]^{2+}$	2	P	B, 2	136
$[\mathrm{Pt^{II}(ado)_2(NH_3)_2)}]^{2+}$	2	P	B, 2	136
$[\mathrm{Pt^{II}(ado)_2(en)}]^{2+}$	2	P	B, 2	136
$[\mathrm{Pt^{II}(gua\text{-}DNA)(NH_3)_3}]^{2+}$	1	N	B, 2	138
$[\mathrm{Pt^{II}(ade\text{-}DNA)(NH_3)_3}]^{2+}$	1	N	B, 2	138
$[\mathrm{Pt^{II}(gua\text{-}DNA)_2(NH_3)_2}]^{2+}$	1	N	A, 12	95
$[\mathrm{Pt^{II}(gua\text{-}DNA)_2(NH_3)_2}]^{2+}$	1	N	A, 12	96
$[\mathrm{Pt^{II}(gua\text{-}DNA)_2(NH_3)_2}]^{2+}$	1	N	B, 2	130
$[\mathrm{Pt^{II}(gua\text{-}DNA)_2(NH_3)_2}]^{2+}$	1	P	A, 12	97
$[\mathrm{Pt^{II}(gua\text{-}DNA)_2(NH_3)_2}]^{2+}$	1	P	A, 1	101

TABLE 1 (*continued*)

Complex	No. of structures	Report parameters[a]	Force field software[b]	Ref.
$[\mathrm{Pt^{II}(gua\text{-}DNA)(ade\text{-}DNA)(NH_3)_2}]^{2+}$	2	N	B, 2	135
$[\mathrm{Pt^{II}(gua\text{-}DNA)(ade\text{-}DNA)(NH_3)_2}]^{2+}$	2	N	B, 2	138
$[\mathrm{Pt^{II}(gua\text{-}DNA)(ade\text{-}DNA)(NH_3)_3}]^{2+}$	1	N	B, 2	138
$[\mathrm{Pt^{II}(gua\text{-}DNA)_2(en)}]^{2+}$	2	N	B, 2	130
$[\mathrm{Pt^{II}(gua\text{-}DNA)_2(chxn)}]^{2+}$	3	N	B, 2	130
$[\mathrm{Ra(18C6)(dbp)_2(OH_2)}]^{0}$	1	N	C, 18	152
$[\mathrm{La^{III}(OH_2)_9}]^{3+}$	1	C	B, 17	144
$[\mathrm{La^{III}(OH_2)_5(NO_3)_3}]^{0}$	1	C	B, 17	144
$[\mathrm{La^{III}(OH_2)_2(NO_3)_5}]^{2-}$	2	C	B, 17	144
$[\mathrm{La^{III}(NO_3)_6}]^{3-}$	1	C	B, 17	144
$[\mathrm{Ce^{III}(OH_2)_9}]^{3+}$	1	C	B, 17	144
$[\mathrm{Ce^{III}(OH_2)_5(NO_3)_3}]^{0}$	1	C	B, 17	144
$[\mathrm{Ce^{III}(NO_3)_5}]^{2-}$	1	C	B, 17	144
$[\mathrm{Ce^{III}(NO_3)_6}]^{3-}$	1	C	B, 17	144
$[\mathrm{Pr^{III}(OH_2)_9}]^{3+}$	2	C	B, 17	144
$[\mathrm{Pr^{III}(OH_2)_4(NO_3)_3}]^{0}$	1	C	B, 17	144
$[\mathrm{Nd^{III}(OH_2)_9}]^{3+}$	2	C	B, 17	144
$[\mathrm{Nd^{III}(OH_2)_4(NO_3)_3}]^{0}$	1	C	B, 17	144
$[\mathrm{Nd^{III}(OH_2)(NO_3)_5}]^{2-}$	1	C	B, 17	144
$[\mathrm{Nd^{III}(NO_3)_6}]^{3-}$	1	C	B, 17	144
$[\mathrm{Sm^{III}(OH_2)_9}]^{3+}$	2	C	B, 17	144
$[\mathrm{Sm^{III}(OH_2)(NO_3)_5}]^{2-}$	1	C	B, 17	144
$[\mathrm{Eu^{III}(OH_2)_9}]^{3+}$	1	C	B, 17	144
$[\mathrm{Eu^{III}(dmp)_3(quin)}]^{0}$	1	C	B, 3	140
$[\mathrm{Eu^{III}(dmp)_3(quin)}]^{0}$	1	C	B, 3	141
$[\mathrm{Eu^{III}(dmp)_3(dmto)}]^{0}$	1	C	B, 3	141
$[\mathrm{Gd^{III}(OH_2)_8}]^{3+}$	2	C	B, 17	144
$[\mathrm{Gd^{III}(OH_2)_9}]^{3+}$	1	C	B, 17	144
$[\mathrm{Gd^{III}(OH_2)_3(NO_3)_3}]^{0}$	2	C	B, 17	144
$[\mathrm{Tb^{III}(OH_2)_9}]^{3+}$	1	C	B, 17	144
$[\mathrm{Dy^{III}(OH_2)_8}]^{3+}$	1	C	B, 17	144
$[\mathrm{Dy^{III}(OH_2)_9}]^{3+}$	1	C	B, 17	144
$[\mathrm{Dy^{III}(OH_2)_3(NO_3)_3}]^{0}$	2	C	B, 17	144
$[\mathrm{Ho^{III}(OH_2)_9}]^{3+}$	1	C	B, 17	144
$[\mathrm{Ho^{III}(NO_3)_5}]^{2-}$	1	C	B, 17	144
$[\mathrm{Er^{III}(OH_2)_9}]^{3+}$	1	C	B, 17	144
$[\mathrm{Er^{III}(NO_3)_5}]^{2-}$	1	C	B, 17	144
$[\mathrm{Tm^{III}(OH_2)_9}]^{3+}$	1	C	B, 17	144
$[\mathrm{Yb^{III}(OH_2)_9}]^{3+}$	2	C	B, 17	144
$[\mathrm{Yb^{III}(acac)_3(OH_2)}]^{0}$	2	C	B, 3	140
$[\mathrm{Yb^{III}(acac)_3(OH_2)}]^{0}$	2	C	B, 3	141
$[\mathrm{Lu^{III}(OH_2)_8}]^{3+}$	2	C	B, 17	144
$[\mathrm{Lu^{III}(OH_2)_9}]^{3+}$	1	C	B, 17	144

TABLE 1 (*continued*)

Complex	No. of structures	Report parameters[a]	Force field software[b]	Ref.
[M(en)]	1	N	A, 1	67
[M(en)$_3$]	1	N	A, 1	43
[M(tn)]	1	N	A, 1	67
[M(trien)]	1	N	A, 1	67
[M(2,3,2-tet)]	1	N	A, 1	67
[M(9aneN$_3$)$_2$]	1	C	A, 7	62
[M(9aneS$_3$)$_2$]	1	C	A, 7	62
[M(12aneN$_4$)]	1	N	A, 4	21
[M(12aneN$_4$)]	1	N	A, 1	44
[M(12aneN$_4$)]	3	N	A, 1	55
[M(12aneN$_4$)]	1	N	A, 1	58
[M(1,4-C$_2$-12aneN$_4$)]	1	P	A, 7	63
[M(13aneN$_4$)]	1	N	A, 4	21
[M(13aneN$_4$)]	1	N	A, 1	44
[M(13aneN$_4$)]	4	N	A, 1	55
[M(14aneN$_4$)]	1	N	A, 4	21
[M(14aneN$_4$)]	1	N	A, 1	44
[M(14aneN$_4$)]	5	N	A, 1	55
[M(14aneN$_4$)]	1	N	A, 1	58
[M(Me$_2$Py-14aneN$_4$)]	1	N	A, 3	86
[M(Me$_2$Py-14aneN$_4$)(NO$_2$)$_2$]	1	N	A, 3	86
[M(Me$_2$Py-14aneN$_4$)(en)]	1	N	A, 3	86
[M(Me$_2$Py-14dieneN$_4$)]	1	N	A, 3	86
[M(15aneN$_4$-1)]	1	N	A, 4	21
[M(Me$_2$Py-15aneN$_5$)]	2	P	A, 3	84
[M(Me$_2$Py-15aneN$_5$)(Cl)]	1	P	A, 3	84
[M(Me$_2$Py-15aneN$_5$)(Cl)$_2$]	1	P	A, 3	84
[M(Me$_2$Py-15dieneN$_5$)(NCS)$_2$]	1	P	A, 3	89
[M(16aneN$_4$)]	1	N	A, 4	21
[M(Me$_2$Py-16dieneN$_5$)(NCS)$_2$]	1	P	A, 3	89
[M(porphyrin-1)]	1	P	A, 11	104
[M(porphyrin-3)]	2	P	A, 10	100
[M(porphyrin-5)]	1	P	A, 11	104
[M(porphyrin-6)]	1	P	A, 11	104
[M(porphyrin-7)]	1	P	A, 11	104
[M(porphyrin-8)]	1	P	A, 11	104
[M(porphyrin-9)]	1	P	A, 11	104
[M(Me$_2$Py-17dieneN$_5$)(NCS)$_2$]	1	P	A, 3	89
[M(18C6)(Cl)$_2$]	1	P	A, 3	87
[M(B$_2$Py$_2$-18tetraeneN$_4$O$_2$)(Cl)$_2$]	1	P	A, 3	90
[M(20tetraeneN$_4$O$_2$)(OH$_2$)$_2$]	1	P	A, 3	88
[M(sar)]	6	N	B, 2	133
[M(CO)$_4$]	2	C	B, n.a.	139
[M(CO)$_5$]	2	C	B, n.a.	139
[M(CO)$_6$]	2	C	B, n.a.	139

TABLE 1 (*continued*)

Complex	No. of structures	Report parameters[a]	Force field software[b]	Ref.
$[M(CO)_7]$	3	C	B, n.a.	139
$[M(Cp)_2]$	1	N	B, 7	142
$[M(Cp)_2(CO)_2]$	1	N	B, 7	142
$[M(Cp)_2(CO)_2]$	1	N	B, 7	143
$[M(Cp)_2(H)_2]$	1	N	B, 7	143
$[M(Cp)_2(Cl)_2]$	1	N	B, 7	142
$[M(Cp)_2(Cl)_2]$	1	N	B, 7	143
$[M(Me_5Cp)_2(CO)_2]$	1	N	B, 7	142
$[M(Me_5Cp)_2(CO)_2]$	1	N	B, 7	143
$[M(Cp)_2(CO)_3]$	1	N	B, 7	142
$[M(Cp)_2(H)_3]$	1	N	B, 7	142
$[M(Cp)_2(H)_3]$	1	N	B, 7	143
$[M(Cp)_2(CO)_4]$	1	N	B, 7	142
$[M(C_4H_4)_2(CO)_3]$	1	N	B, 7	142

[a] The reporting of parameters is coded as follows: C, a complete parameter set is given; P, a partial set of parameters for use with another force field are given; N, no parameters are presented.

[b] The type of force field is coded as follows: A, valence force field method; B, points-on-a-sphere method; C, ionic method. Software is coded as follows: 1, modified version of Boyd's 1968 program; 2, the MOMEC program; 3, modified version of the MM2 program; 4, Boyd's 1968 program; 5, the CFF program; 6, modified version of Wiberg program; 7, the MOLBLD program; 8, the MOLMEC program; 9, modified version of the MODEL program; 10, the MacroMODEL program; 11, the BIOGRAF program; 12, the AMBER program; 13, the YETI program; 14, modified version of the CHARMM program; 15, the AGNAS program; 16, the MMPP program; 17, the MM2 program; 18, the WMIM program; n.a., information not available.

both those who desire to try their hand at such calculations and those who have already contributed to the field. The compilation is intended to be an exhaustive one and has been designed to allow a potential user to quickly determine whether calculations have previously been performed on a given metal ion and/or ligand. To accomplish this goal, the compilation of calculations has been organized in two ways.

One way to organize the calculations is by the identity of the metal ion in the complex. This has been done in Table 1 where the entries for all calculations on each metal ion species are grouped together. These groups are arranged in order of the atomic number of the metal. Calculations that have been performed on complexes that contain a generic metal ion, M, have been included at the end of the table. Each entry in the table consists of an abbreviated formula for the metal complex and some additional information concerning the calculation. The ligand abbreviations that are used in the table can be understood by referring to the structures and names that are given in Scheme 1. The additional information in each entry includes the number

NH_3

Co^{III}, 25, 42, 47, 53, 57, 61, 92, 118, 119, 120, 131; Co^{II}, 131; Ni^{II}, 53, 92; Pt^{II}, 95, 101, 130, 135, 136, 138.

CH_3NH_2

Co^{III}, 53

quin

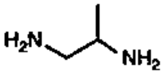
Eu^{III}, 140, 141

CH_3CN

Cu^{II}, 88

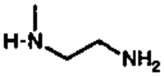
en

Co^{III}, 13, 14, 19, 24, 49, 53, 61, 72, 73, 77, 83, 92, 131; Co^{II}, 49, 131; Ni^{II}, 35, 37, 38, 53, 63, 86, 92; Pt^{II}, 130, 136; M, 8, 43.



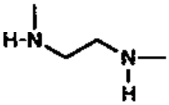
pn

Co^{III}, 14, 19, 75, 119, 129; Co^{II}, 129.



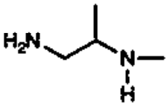
N-Meen

Co^{III}, 19.



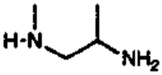
N,N'-Me$_2$en

Co^{III}, 19.



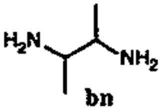
N$_1$-Mepn

Co^{III}, 19.



N$_2$-Mepn

Co^{III}, 19.

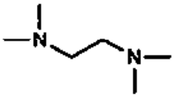


bn

Co^{III}, 19, 41, 72, 73, 74.

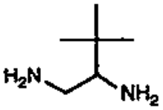
ibn

Co^{III}, 73, 74.



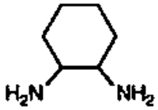
tmen

Pt^{II}, 136.



dmbn

Co^{III}, 119.

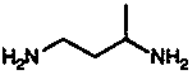


chxn

Co^{III}, 75; Pt^{II}, 130.

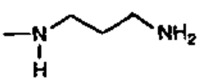
tn

Co^{III}, 12, 18, 19, 53, 69, 71, 77, 92, 131; Co^{II}, 131; Ni^{II}, 35, 37, 53; M, 8.



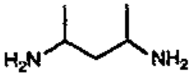
1,3-bn

Co^{III}, 19.



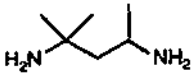
N-Metn

Co^{III}, 19.



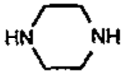
ptn

Co^{III}, 69, 70, 71, 77, 118.



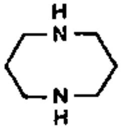
mptn

Co^{III} & Pt^{II}, 120;



pip

Co^{III}, 92.

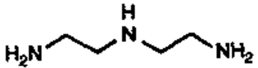


daco

Ni^{II}, 52, 53, 63.

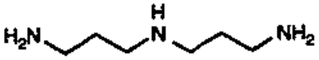
tmd

Co^{III}, 92.



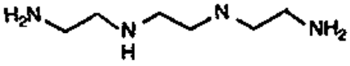
dien

Co^{III}, 15, 18, 27, 29, 61, 92, 122, 123, 125, 131; Co^{II}, 125, 131; Ni^{II}, 35, 37, 38, 53, 92.



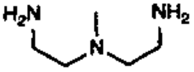
dpt

Co^{III}, 13, 92, 121, 122, 123, 131; Co^{II}, 131; Ni^{II}, 35, 37, 53.



trien

Co^{III}, 10, 11, 14, 23, 24, 26, 42, 57, 61, 92, 126; Ni^{II}, 37, 38, 92; M, 67.

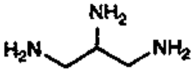


dema

Co^{III}, 29.

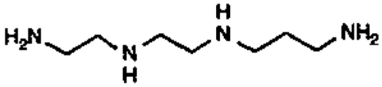
2,3,2-tet

Co^{III}, 126; Ni^{II}, 37, 44; M, 67.



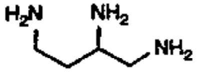
1,2,3-pn

Co^{III}, 53, 131, 132; Co^{II}, 131.



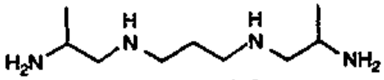
2,2,3-tet

Co^{III}, 36.



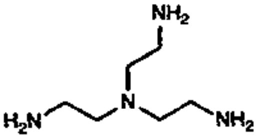
trab

Co^{III}, 134.



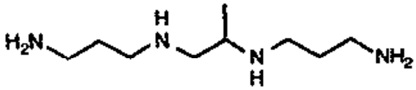
2,10-Me$_2$-2,3,2-tet

Co^{III}, 39, 40.



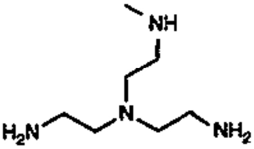
tren

Co^{III}, 25, 28.



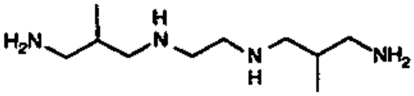
5-Me-3,2,3-tet

Co^{III}, 20.



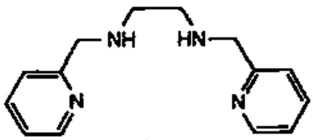
Metren

Co^{III}, 47.



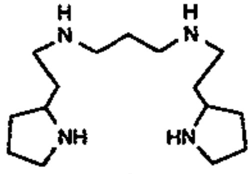
3,10-Me$_2$-3,2,3-tet

Co^{III}, 50.



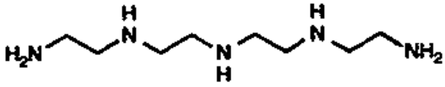
picpn

Co^{III}, 17, 22.



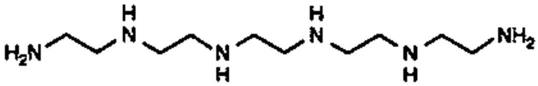
pyht

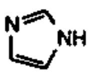
Co^{III}, 39.

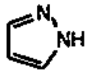


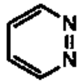
tetraen

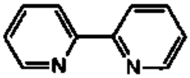
Co^{III}, 16, 61, 92; Ni^{II}, 38.

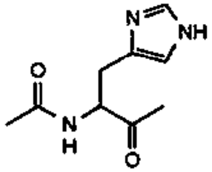

pentaen
Co^{III}, 27, 92; Ni^{II}, 38.

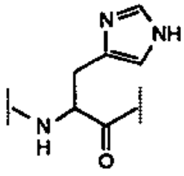

imd
Fe^{II}, 65;
Zn^{II}, 98.

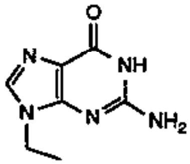

pyz
Cu^{II}, 88.

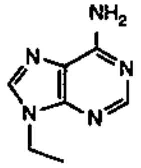

pydz
Cu^{II}, 88.

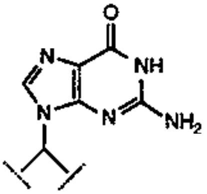

bpy
Pt^{II}, 120.

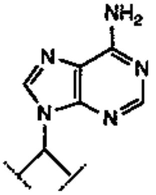

R-imd
Zn^{II}, 98.

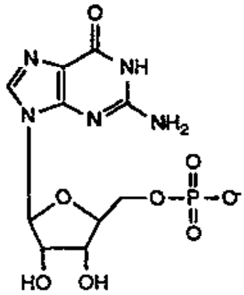

his-CA
Zn^{II}, 151, 162-165.


9-Etgua
Pt^{II}, 136.

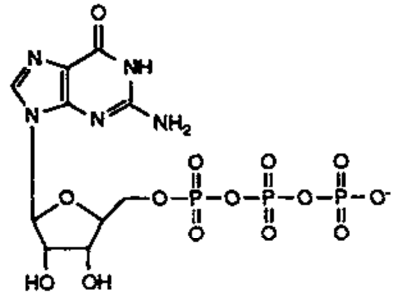

9-Etade
Pt^{II}, 136.


gua-DNA
Pt^{II}, 95, 96, 97,
101, 130, 135.

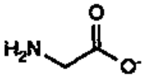

ade-DNA
Pt^{II}, 135, 138.



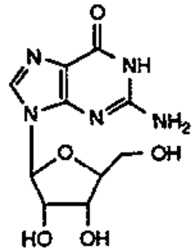
5'-gmp
$\mathrm{Pt^{II}}$, 137.



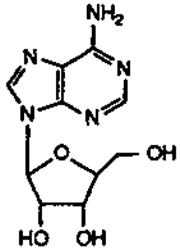
5'-gtp
$\mathrm{Pt^{II}}$, 137.



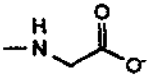
glyO
$\mathrm{Co^{III}}$, 14, 22,
23, 26, 28.



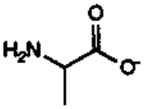
guo
$\mathrm{Pt^{II}}$, 136.



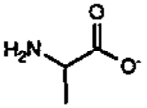
ado
$\mathrm{Pt^{II}}$, 136.



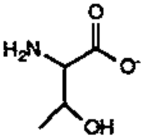
N-MeglyO
$\mathrm{Co^{III}}$, 14, 24.



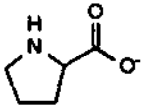
alaO
$\mathrm{Co^{III}}$, 22, 39.



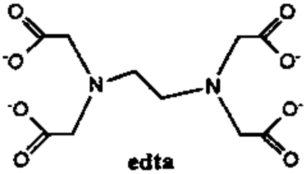
N-MealaO
$\mathrm{Co^{III}}$, 11, 24, 40.



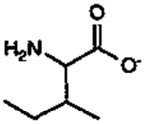
thrO
$\mathrm{Cu^{II}}$, 78.



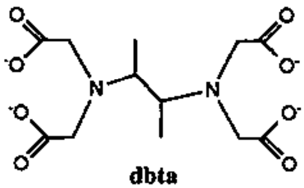
proO
$\mathrm{Co^{III}}$, 10, 14.



edta
$\mathrm{Co^{III}}$, 32.

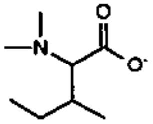


ileuO
$\mathrm{Cu^{II}}$, 78.



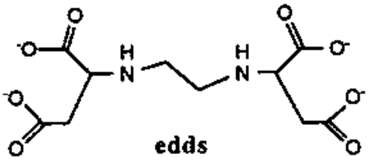
dbta

Co^{III}, 48.



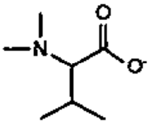
N,N-Me$_2$ileuO

Cu^{II}, 80.



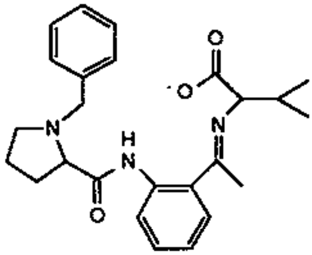
edds

Co^{III}, 33.



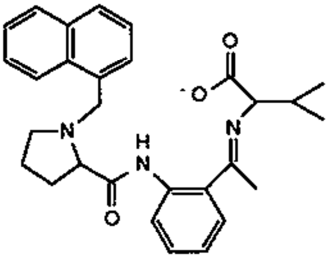
N,N-Me$_2$valO

Cu^{II}, 79, 81, 82.



BPAAP-valO

Ni^{II}, 59.



NPAAP-valO

Ni^{II}, 64.

H_2O

Ni^{II}, 37, 38, 62, 107; Cu^{II}, 56; Zn^{II}, 98, 151, 162-165; Rh^{II}, 66; Ia metals, 145, 155; IIa metals, 88, 152; lanthanides, 140, 141, 144.

OH^-

Zn^{II}, 98.

O^{2-}

Rh^{II}, 60.

O_2

Fe^{II}, 65.

CH_3OH

Ia metals, 148.

HCO_3^-

Zn^{II}, 151, 162-165

CO_3^{2-}

Co^{III}, 12, 18, 53.

NO_2^-

Co^{III}, 53; Ni^{II}, 86.

NO_3^-

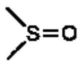
lanthanides, 144.

S^{2-}

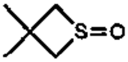
Rh^{II}, 60.

SCN^-

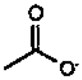
Cu^{II}, 88; Ni^{II}, 89; M, 105.



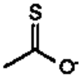
Rh^{II}, 66.



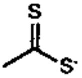
dmto
Eu^{III}, 141.



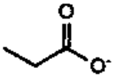
Rh^{II}, 60, 66; Cu^{II},
Cd^{II}, & Pd^{II}, 60.



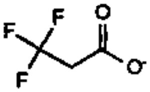
Rh^{II}, 60.



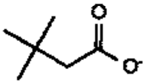
Rh^{II} & Pd^{II}, 60.



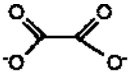
Rh^{II}, 66.



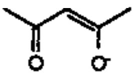
Rh^{II}, 66.



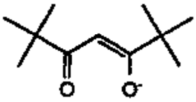
Rh^{II}, 66.



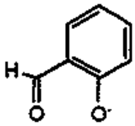
ox
Co^{III}, 17.



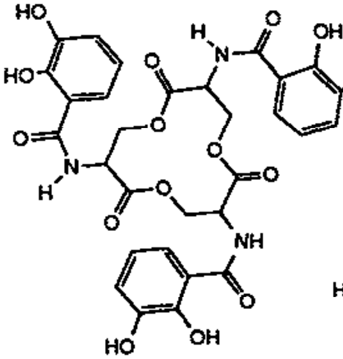
acac
Yb^{III}, 140, 141



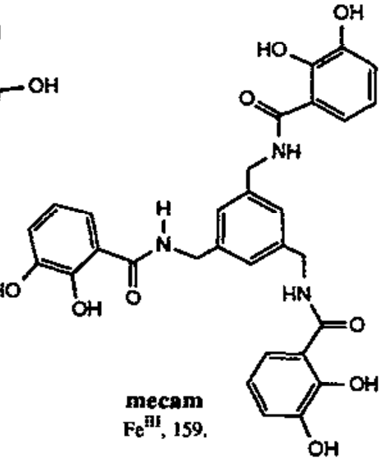
dmp
Eu^{III}, 140, 141.



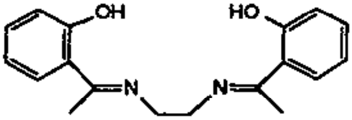
sal
Co^{III}, 91.



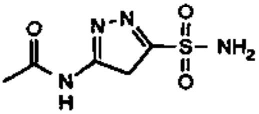
enterobactin
Fe^{III}, 159.



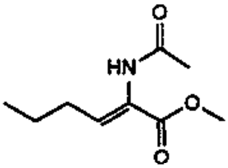
mecam
Fe^{III}, 159.



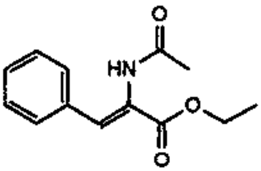
Me_2sal_2tn
Co^{III}, 91.



RSO_2NH_2
Zn^{III}, 151, 162-165.



aaa
Rh^{I}, 108.



aac
Rh^{I}, 108.

Cl$^-$
Co^{III}, 9, 13, 16, 20, 25, 30, 31, 47, 50, 53, 93, 126; M, 142, 143.

CO
Fe^{II}, 65; Cr^{0}, 102, 103; M, 139, 142, 143.

CN$^-$
Co^{III}, 120.

H$^-$
M, 142, 143.

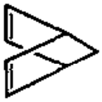
CH_3
Co^{III}, 93, 94..

C_4H_4
M, 142.

cp
M, 142, 143.

Me_5cp
M, 142, 143.

cod
Rh^{I}, 108.



nbd
Rh^{I}, 108.

PMe_3
Rh^{I}, 166; Cr^{0}, 103.

PMe_2Et
Cr^{0}, 103.

PMe_2(*i*-Pr)
Cr^{0}, 103.

PMe_2(*t*-Bu)
Cr^{0}, 103.

$PMeEt_2$
Cr^{0}, 103.

PMe(*i*-Pr)$_2$
Cr^{0}, 103.

PMe(*t*-Bu)$_2$
Cr^{0}, 103.

$PMePh_2$
Rh^{I}, 108.

PEt_3
Cr^{0}, 103.

PEt_2(*i*-Pr)
Cr^{0}, 103.

PEt_2(*t*-Bu)
Cr^{0}, 103.

PEt(*i*-Pr)$_2$
Cr^{0}, 103.

PEt(*t*-Bu)$_2$
Cr^{0}, 103.

P(*i*-Pr)$_3$
Cr^{0}, 103.

P(*i*-Pr)$_2$(*t*-Bu)
Cr^{0}, 103.

P(*i*-Pr)(*t*-Bu)$_2$
Cr^{0}, 103.

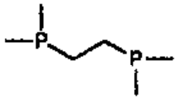
P(*t*-Bu)$_3$
Cr^{0}, 103.

P(*n*-Bu)$_3$
Cr^{0}, 103.

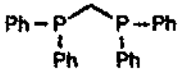
P(*i*-Bu)$_3$
Cr^{0}, 103.

P(cy)$_3$
Cr^{0}, 103.

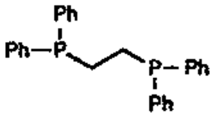
PPh_3
Cd^{II}, 60.



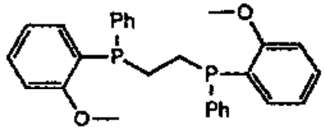
dmpe
Rh^{I}, 108.



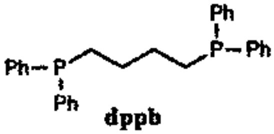
dppm
Cu^{II}, 88.



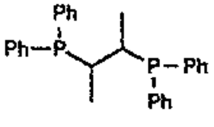
dmpe
Rh^{I}, 108.



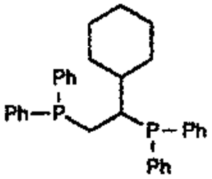
dipamp
Rh^{I}, 108.



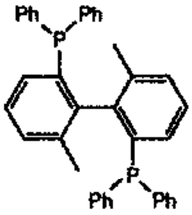
dppb
Rh^{I}, 108.



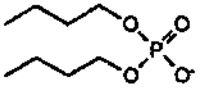
chphos
Rh^{I}, 108.



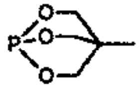
cycphos
Rh^{I}, 108.



bdpbp
Rh^{I}, 108.



dbp
IIa metals, 152.



$P(OCH_2)_3CMe$
Cr^{0}, 102.

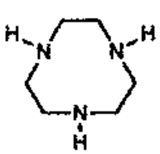
$P(OMe)_3$
Cr^{0}, 102.

$P(OEt)_3$
Cr^{0}, 102.

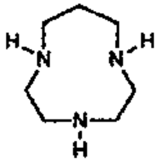
$P(O(i\text{-}Pr))_3$
Cr^{0}, 102.

$P(OPh)_3$
Cr^{0}, 102.

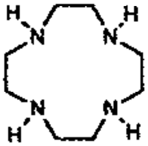
$P(O(t\text{-}Bu))_3$
Cr^{0}, 102.



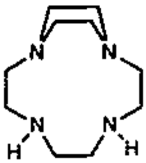
9aneN$_3$
Co^{III}, 53, 131; Co^{II}, 131;
Ni^{II}, 53, 62; M, 62.



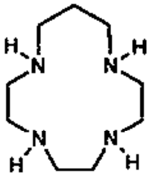
10aneN$_3$
Co^{III}, 46.



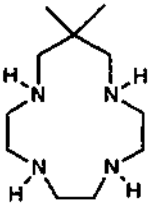
12aneN$_4$
Co^{III}, 53; M, 21,
44, 55, 58.



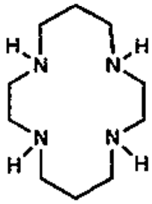
1,4-C_2-12aneN$_4$
Ni^{II}, 63, 106.



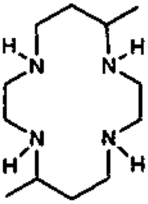
13aneN$_4$
Co^{III}, 30, 31 126; Ni^{II},
63; M, 21, 44, 55.



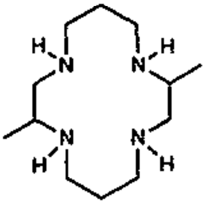
Me$_2$-13aneN$_4$
Ni^{II}, 106.



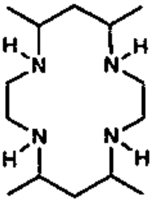
14aneN$_4$
Co^{III}, 30, 31, 94, 126;
Ni^{II}, 44, 106; M, 21,
44, 55, 58.



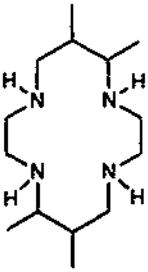
Me$_2$-14aneN$_4$-1
Ni^{II}, 63, 106.



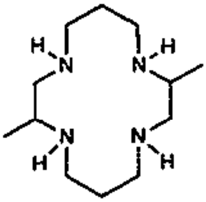
Me$_2$-14aneN$_4$-2
Ni^{II}, 106.



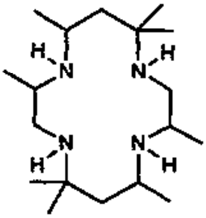
Me$_4$-14aneN$_4$-1
Ni^{II}, 106.



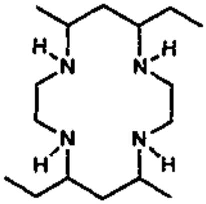
Me$_4$-14aneN$_4$-2
Ni^{II}, 106.



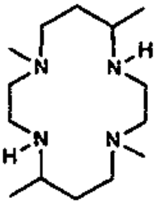
Me$_6$-14aneN$_4$
Ni^{II}, 106.



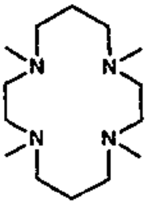
Me$_8$-14aneN$_4$
Ni^{II}, 106.



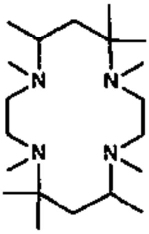
Me$_2$Et$_2$-14aneN$_4$
Ni^{II}, 106.



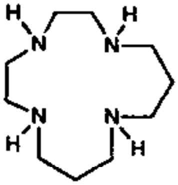
Me$_2$-DMC
Ni^{II}, 106.



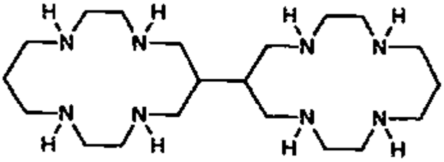
TMC
Ni^{II}, 63, 99, 106,
124, 128.



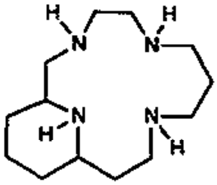
Me$_6$-TMC
Ni^{II}, 106.



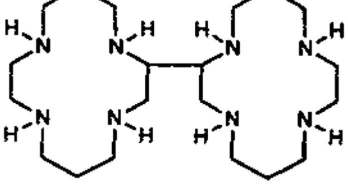
isocyclam
Ni^{II}, 51.



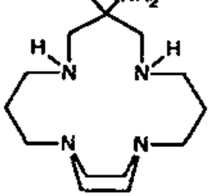
(14aneN$_4$)$_2$-1
Ni^{II}, 106.



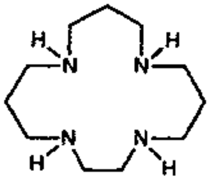
chxn-14aneN$_4$
Ni^{II}, 106.



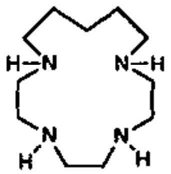
(14aneN$_4$)$_2$-2
Ni^{II}, 106.



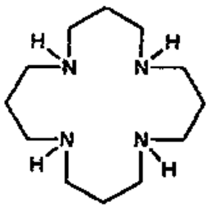
Me(NH$_2$)(1,4-C$_2$)15aneN$_4$
Co^{III}, 68.



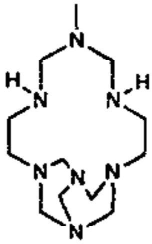
15aneN$_4$-1
Co^{III}, 30, 31,
126; *M*, 21.



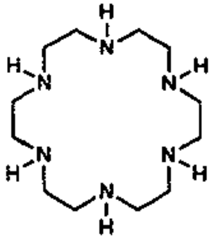
15aneN$_4$-2
Ni^{II}, 106.



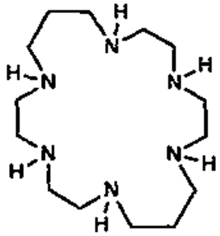
16aneN$_4$
Co^{III}, 30, 31,
126; M, 21.



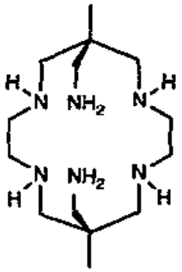
cap,Me-14aneN$_6$
Ni^{II}, 106.



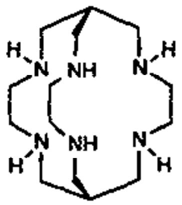
18aneN$_6$
Co^{III}, 34, 92.



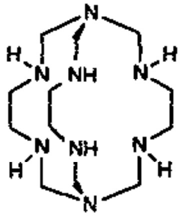
20aneN$_6$
Co^{III}, 45.



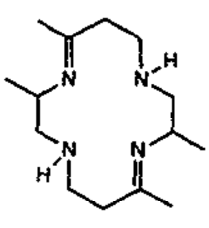
diammac
Co^{III} & Co^{II}, 131.



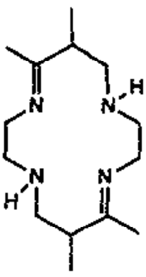
sar
Co^{III}, 131, 133;
Co^{II}, 131; M, 133.



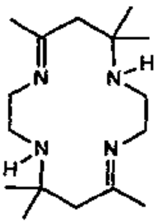
sep
Co^{III} & Co^{II}, 49,
125, 131.



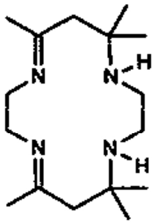
Me$_4$-14dieneN$_4$-1
Ni^{II}, 106.



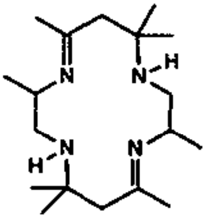
Me$_4$-14dieneN$_4$-2
Ni^{II}, 106.



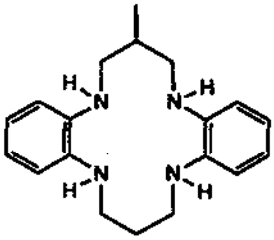
Me$_6$-14dieneN$_4$-1
Co^{III}, 93, 94; Ni^{II}, 106.



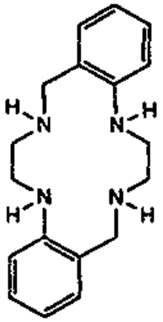
Me$_6$-14dieneN$_4$-2
Ni^{II}, 106.



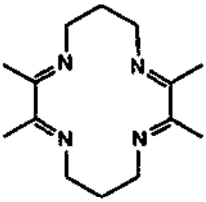
Me$_8$-14dieneN$_4$
Ni^{II}, 106.



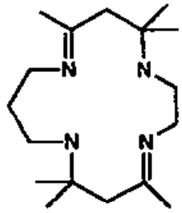
B$_2$Me-14dieneN$_4$
Ni^{II}, 105.



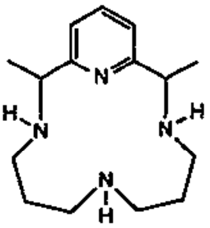
B$_2$-14dieneN$_4$
Ni^{II}, 105.



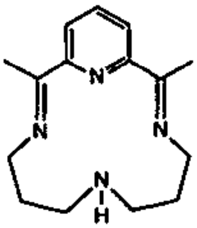
Me$_4$-14tetraeneN$_4$
Co^{III}, 94.



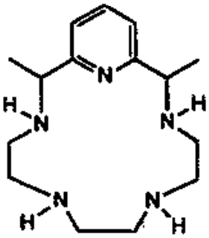
Me$_6$-15dieneN$_4$
Ni^{II}, 106.



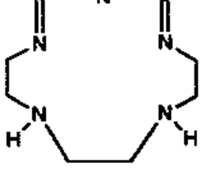
Me$_2$Py-14aneN$_4$
Ni^{II} & M, 86.



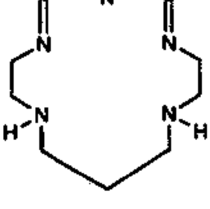
Me$_2$Py-14dieneN$_4$
Ni^{II}, 86.



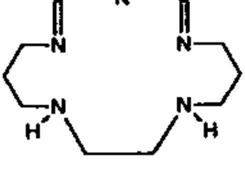
Me$_2$Py-15aneN$_5$
M, 84.



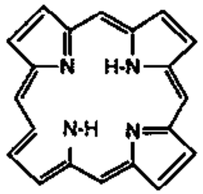
Me$_2$Py-15dieneN$_5$
M, 89.



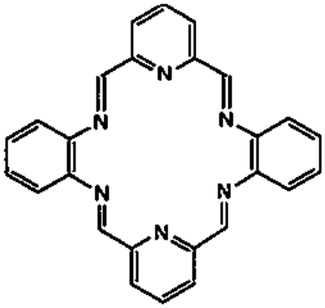
Me$_2$Py-16dieneN$_5$
M, 89.



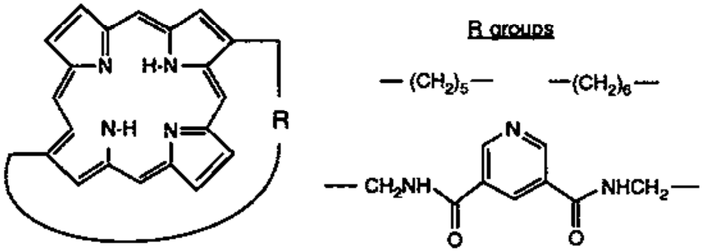
Me$_2$Py-17dieneN$_5$
M, 89.



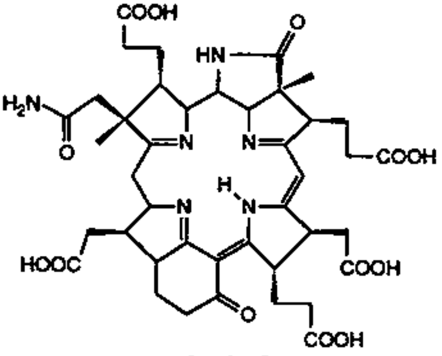
porphyrin-1
Ni^{II}, Fe^{II}, Zn^{II}, Pb^{II}, 65;
M, 104.



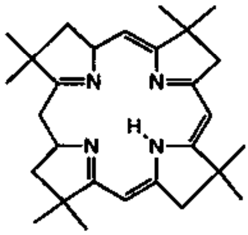
B$_2$Py$_2$-18tetraeneN$_6$
M, 90.



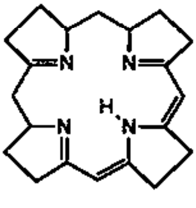
porphyrin-2
Fe^{II}, 65.



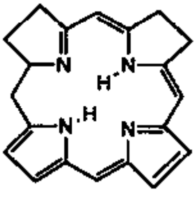
porphyrin-3
Ni^{II}, M, 100.



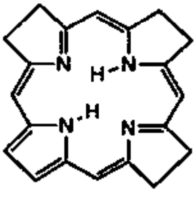
porphyrin-4
Ni^{II}, 104.



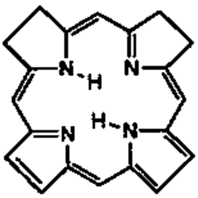
porphyrin-5
M, 104.



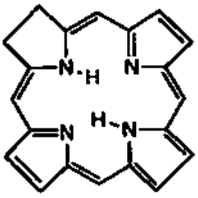
porphyrin-6
M, 104.



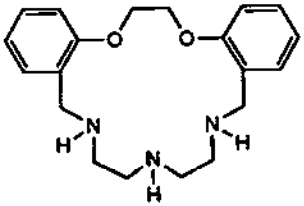
porphyrin-7
M, 104.



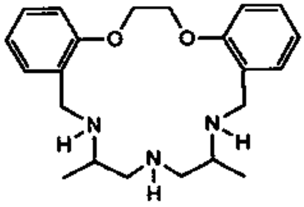
porphyrin-8
M, 104.



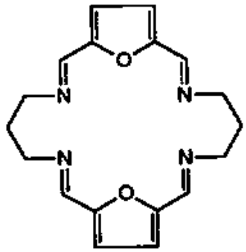
porphyrin-9
M, 104.



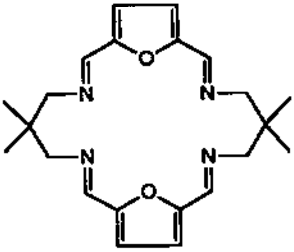
B_2-17dieneN$_3$O$_2$
Ni^{II}, 107.



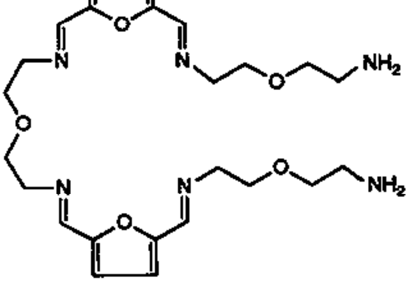
Me$_2$B$_2$-17dieneN$_3$O$_2$
Ni^{II}, 107.



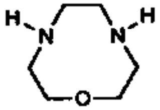
20tetraeneN$_4$O$_2$
Cu^{II} & Ba^{II}, 88.



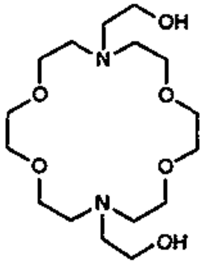
Me$_4$-20tetraeneN$_4$O$_2$
Cu^{II}, 88.



N$_6$O$_6$ podand
Cu^{II}, 85.

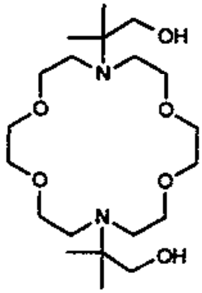


9aneN$_2$O
Ni^{II}, 54.



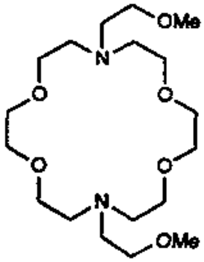
18aneN$_2$O$_4$-1

K$^+$, 150.



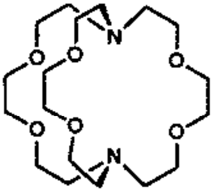
18aneN$_2$O$_4$-2

K$^+$, 150.



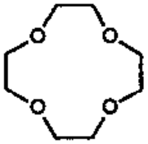
18aneN$_2$O$_4$-3

K$^+$, 150.



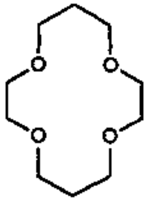
2,2,2-crypt

Na$^+$, K$^+$, Rb$^+$, Cs$^+$, 146.



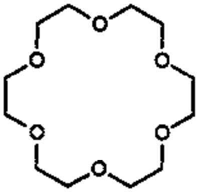
12C4

Li$^+$,Na$^+$, K$^+$, 67.



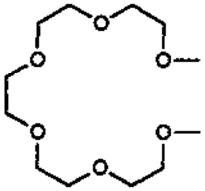
14C4

Li$^+$,Na$^+$, K$^+$, 67.



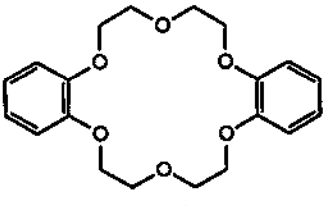
18C6

Li$^+$, 153; Na$^+$, 145, 153, 155; K$^+$, 145, 153, 154, 155; Rb$^+$, 145, 155; Cs$^+$, 145, 155; Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, & Ra^{2+}, 152; M, 87.



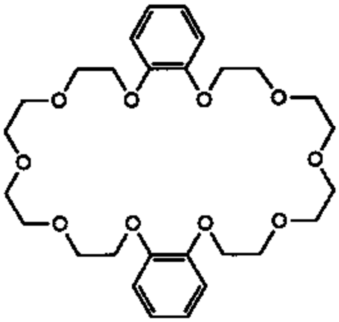
pentaglyme

Na$^+$, K$^+$, Rb$^+$, Cs$^+$, 145.



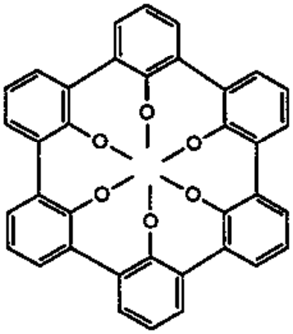
B_218C6

Li^+, Na^+, K^+, Rb^+, Cs^+, 148.



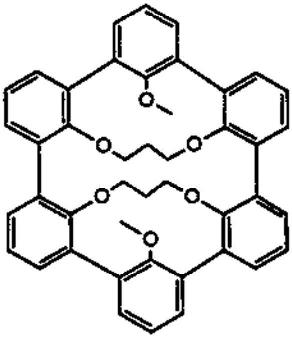
B_230C10

Li^+, Na^+, K^+, Rb^+, Cs^+, 148.



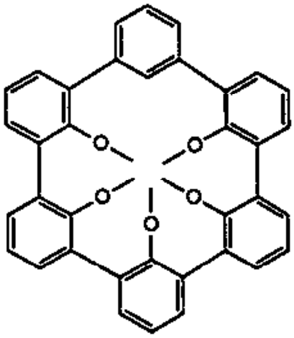
spherand-1

Li^+, Na^+, K^+, 147.



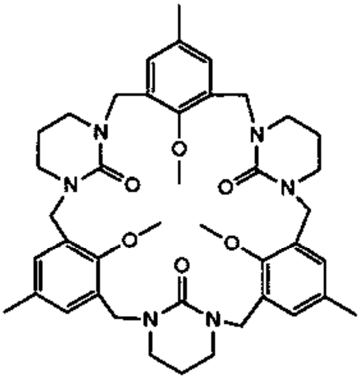
spherand-3

Li^+, Na^+, 147.



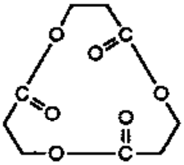
spherand-2

Li^+, Na^+, K^+, 147.



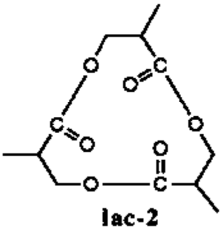
spherand-4

Li^+, Na^+, K^+, Rb^+, Cs^+, 149.



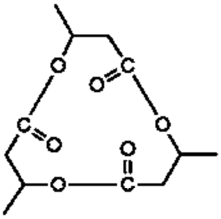
lac-1

Li^+, Na^+, K^+, 156.



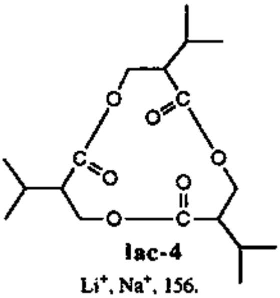
lac-2

Li^+, Na^+, K^+, 156.



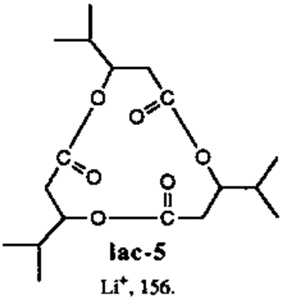
lac-3

Li^+, Na^+, K^+, 156.



lac-4

Li^+, Na^+, 156.

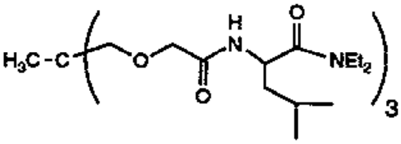


lac-5

Li^+, 156.

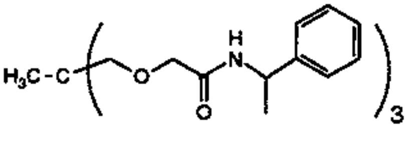
trispep-1

Ca^{2+}, 161.

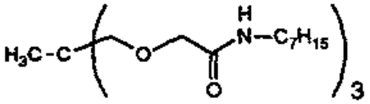


trispep-2

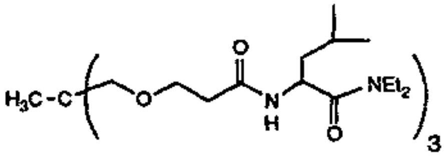
Ca^{2+}, 161.



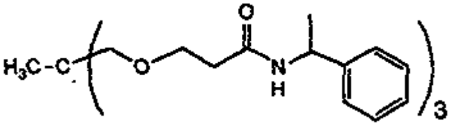
trispep-3
Ca^{2+}, 161.



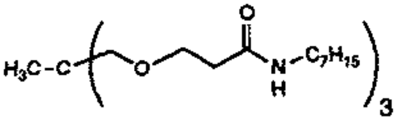
trispep-4
Ca^{2+}, 161.

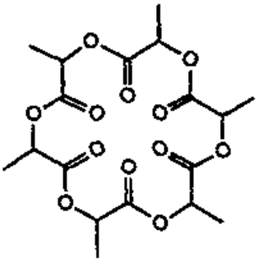


trispep-5
Ca^{2+}, 161.

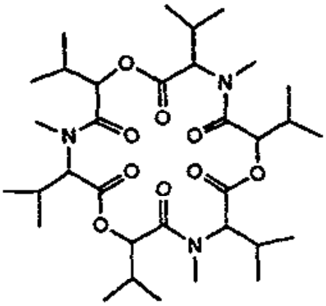


trispep-6
Ca^{2+}, 161.

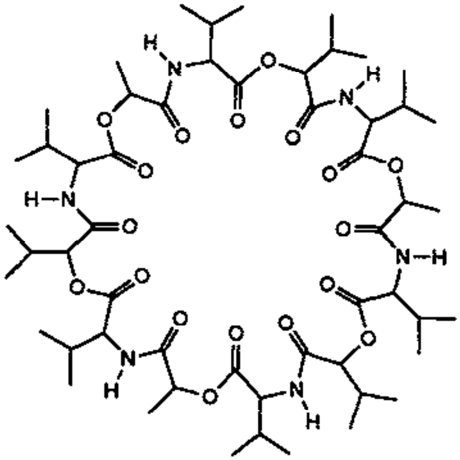




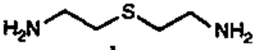
lac-6
Li^+, Na^+, K^+, 156.



enniatinB
Li^+, Na^+, K^+, Rb^+, Cs^+, 157.

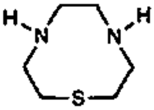


valinomycin
Li^+, Na^+, K^+, Rb^+, Cs^+, 158.

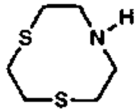


daes
Co^{III}, 75; Cu^{II} & Ni^{II}, 62.

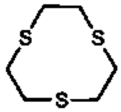
aeaps
Co^{III}, 75.



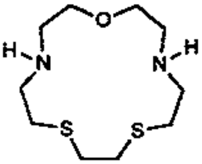
9aneN$_2$S
Cu^{II} & Ni^{II}, 62.



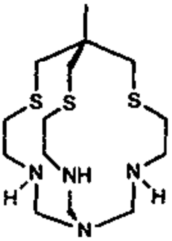
9aneNS$_2$
Ni^{II}, 62.



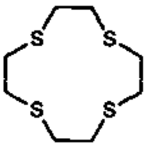
9aneS$_3$
M & Ni^{II}, 62.



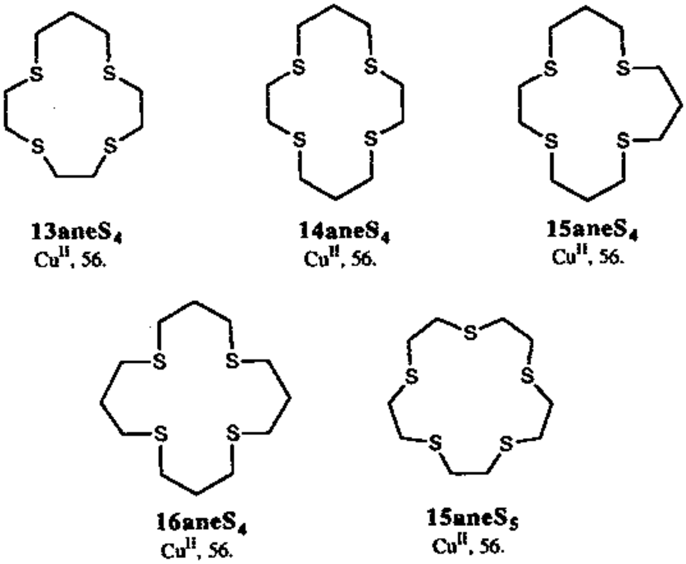
15aneN$_2$OS$_2$
Ni^{II}, 62.



azacapten
Co^{III} & Co^{II}, 127.



12aneS$_4$
Cu^{II}, 56.



13aneS$_4$
Cu^{II}, 56.

14aneS$_4$
Cu^{II}, 56.

15aneS$_4$
Cu^{II}, 56.

16aneS$_4$
Cu^{II}, 56.

15aneS$_5$
Cu^{II}, 56.

Scheme 1. Complexed ligands for which molecular mechanics calculations have been reported. Each entry consists of the structure of a ligand, the abbreviation that was used in Table 1, and references to the calculations that have been done on the ligand.

of structures (conformations, diastereoisomers, etc.) that were calculated for the complex, the extent to which the force field parameters are reported, the type of force field that was used, the code that was used, and a literature reference to the work.

Another way to organize the calculations is by the identity of the ligand. This has been done in Scheme 1. To the extent that it was possible, the ligands have been grouped according to the type of donor atoms that they contain. Each entry in Scheme 1 consists of a structure of the ligand, the abbreviation for the ligand that was used in Table 1, and references to the calculations that have been done on the ligand as a function of metal ion.

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