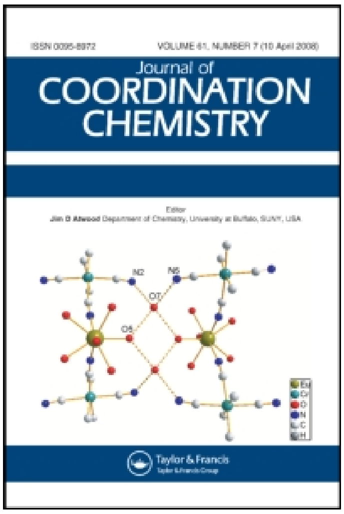

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COBALT-59 NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY IN COORDINATION CHEMISTRY

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The current status of cobalt-59 NMR spectroscopy is reviewed including historical perspectives and application to various areas of coordination chemistry. Chemical shift data are summarized and tabulated for about 800 complexes from values in the literature and our experimental data. Spin–spin coupling constants are also collected for 20 nuclear pairs.

Keywords: Cobalt-59, NMR

1. HISTORICAL

Among the numerous non-zero spin nuclei, cobalt-59 has an important and somewhat characteristic role in the history of nuclear magnetic resonance (NMR).[1–4] In the early stages of NMR (soon after the first discoveries of NMR spectra in 1945), many physicists had eagerly tried to determine the gyromagnetic ratios of various nuclei. The most important report was that of Proctor and Yu,[5] who measured the gyromagnetic ratios of several cobalt(III) complexes with many other nuclei in 1951. They reported that remarkably large differences in gyromagnetic ratios were observed for several tervalent cobalt complexes. This difference in gyromagnetic ratios was named the "chemical shift", but the relative magnitude is about one thousand-times larger than those of protons. Proctor and Yu reported several very important phenomena for cobalt-59 NMR: (a) The range of differences of the gyromagnetic ratios is exceedingly large (almost 1% or much larger). (b) The trend of the increase of gyromagnetic ratio is approximately parallel to the instability of cobalt(III) complexes. (c) The temperature dependence of the gyromagnetic ratio was fairly large in these cobalt complexes and, (d) Doublet spectra were observed for sodium hexanitrocobaltate(III) complex in aqueous solution.

They proposed very important explanations for these differences in gyromagnetic ratios for cobalt-59, namely

(1) The existence of low-lying excited states.
(2) Rapid transitions between the ground state and the above mentioned excited states.
(3) The temperature-sensitive changes in the populations of ground and excited states.
(4) The large difference of shielding constants between the ground and excited states.

Their suggestions seem to be somewhat speculative, but much of them became the foundations for later theoretical treatment of chemical shifts and applications to coordination chemistry.

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There are more than one hundred papers which contain cobalt-59 NMR data, and several relating parameters have been obtained from the NMR spectra of other nuclei, or nuclear quadrupole resonance spectroscopy. The literature compilation[1–128] is shown at the end of this review from the first observations of Proctor and Yu through to the end of 1987.

Although there are several good reviews of cobalt-59 NMR,[1–4] we have found that they contain occasionally some incorrect descriptions which exist mainly in the original papers (erroneous samples, miscalculations, false assignments of coexisting impurity signals, etc.) even in those reported by several famous scientists, and a critical viewpoint should be taken in compiling trustable data collection. We have tried to reexamine the earlier reported data where possible, and to construct a reliable database for cobalt-59 NMR spectroscopy.

2. CHEMICAL SHIFT

2.1. *Griffith–Orgel Plot*

In 1957, Griffith and Orgel[7] gave a valuable explanation of the chemical shift of cobalt-59 based on Proctor and Yu's data. Surprisingly good correlation was observed for the chemical shift and wavelengths of the "first absorption maxima", namely reciprocals of the energy difference of the 3d electronic orbitals. The explanation was based on the second-order paramagnetic contribution to the chemical shift by applying simple crystal-field theory. The chemical shift can be divided into diamagnetic (σ_d) and paramagnetic (σ_p) terms as in the following:

$$\sigma = \sigma_d + \sigma_p$$

$$\sigma_d = (e^2/2mc^2)\sum_k (< \psi_0|(\Sigma(x_k{}^2 + y_k{}^2)/r_k{}^3)|\psi_0>)$$

$$\sigma_p = (e^2/m^2c^2)\sum_n(<\psi_0|\sum_k m_{zk}|\psi_n> \ <\psi_n|(\sum_k m_{zk}/r^3)|\psi_0>/(E_n - E_0))$$

where the symbols are used as ordinary notations.

The dominant term in the paramagnetic terms can be assumed to be the lowest excited state, namely the energy difference in the paramagnetic term is the smallest one. This corresponds to the d–d splitting, which is usually called CFSE (crystal field splitting energy) or LFSE (ligand field splitting energy) in the low-spin type $3d^6$ complexes, which are approximately expressed as the reciprocals of the so-called first absorption maxima.

Chemical shifts can be expressed by the following simplified equations:

$$\sigma = A - B/\Delta = A - B\lambda$$

This means the magnitude of chemical shifts can be correlated with the spectrochemical series, and the observed cobalt-59 chemical shift data supported this theoretical treatment. By this approximation, the assumptions introduced by Proctor and Yu seem unnecessary in explaining the chemical shift data. Soon after their results were published, Freeman, Murray and Richards[8] reported the chemical shift for 14 cobalt(III) complexes. The chemical shift/wavelength of the first absorption maxima plot (Griffith–Orgel plot) was successfully applied to explain their chemical shift data. (Therefore, some researchers have called this plot FMR). This seems to have made a significant impression on many chemists who have been studying heteronuclear NMR, and many reports for heteronuclear NMR contain figures in which the chemical shifts are plotted against wavelengths of the absorption maxima of samples, but the correlation does not seem as good as with cobalt-59 NMR.

The contribution of the higher order paramagnetic term is expected to produce a field-dependent chemical shift. This field dependence is usually negligibly small but it might possibly be observed for nuclei which show a large chemical shift range, and the high-field NMR raises the chemical shift difference frequency. Bendall and Doddrell[67] reported the existence of a small change in chemical shifts for $[Co(acac)_3]$ and $[Co(NH_3)_6]^{3+}$ between the two resonant fields (2.1 T and 0.3 T). However, the direction was opposite to expectation. The reason for this phenomenon still remains unclear.

2.2. *Effect of Electron Cloud Expansion*

Deviation from a straight correlation between the chemical shift and the first absorption maxima was pointed out firstly by Kanekar and his group[17] for complexes with sulfur-donor ligands, such as dithiocarbamate, xanthate and dithiophosphates. Similar results have also been reported by Yamasaki, Yajima, Fujiwara.[22] These deviations are also observed for complexes which have "soft" ligand atoms such as phosphorus,[61,78,118] selenium,[115] arsenic[118] and antimony.[124]

The theoretical treatment of the electronic spectra for these complexes is included in the "nephelauxetic effect", or electron cloud expansion effect for "soft" ligands. The values of the angular contribution (m_{zk}'/r^3) in the Griffith–Orgel approximation for complexes with relatively soft ligand atom groups are assumed to be much different from those of the relatively hard ligand atom groups. The different linear relationships in the Griffith–Orgel plot are well established for these ligand atom groups.

The nephelauxetic constant (orbital reduction factor) was introduced to overcome these complexities by Fujiwara[24] and more precisely by Juranic,[86] and a good relationship was obtained for a wide variety of complexes including many soft ligand atoms.

Juranic later claimed that a different slope (σ/λ) should be applied for each CoL_6 type complex for different L (N, O, C, P, S etc.).[105]

The magnitude of the gradient σ/λ (=chemical shift/wavelength of the first absorption maxima) in the Griffith–Orgel plot enables us to extend the possibilities of cobalt-59 NMR to many different fields in inorganic chemistry. The small differences in electronic states have been customarily characterized by the visible-ultraviolet absorption spectroscopy (d–d transitions). Of course the "diffuse" bands have prevented discrimination of small differences. The magnitude of the ratio is fairly large ca. 30 ppm/nm for complexes of CoN_xO_{6-x} series), and the many small differences in the electronic states can be easily detected, such as solvation shift (medium effect), temperature dependence, ionic association, and discrimination of isotopomers.

The precision of chemical shift measurement of cobalt-59 is about 0.05 ppm for sharp spectra such as in tetracarbonyl- cobaltate(-I) or hexacyanocobaltate(III) using modern NMR spectrometers. This corresponds to a difference of $\lambda_{1\max}$ in the order of 1 pm(!). In the case of broader spectra such as for hexaamminecobalt(III) or tris(ethylenediamine)-cobalt(III) complexes, it is very easy to determine exactly chemical shift differences in the order of 1 ppm. This sensitivity of cobalt-59 NMR enables us to analyze many subtle effects on the surroundings of the cobalt nucleus much more easily than by the customary electronic spectral measurements.

3. EMPIRICAL RULES OF CHEMICAL SHIFT OF OCTAHEDRAL COBALT(III) COMPLEXES

The prediction and estimation of chemical shifts seems to be valuable in applying cobalt-59 NMR to the characterization of various complexes. As direct estimation from the magnetic susceptibility has been tried by Indian research groups,[88] their trials seem to be qualitatively good for a relatively small number of complexes. Simple empirical rules for chemical shifts were established by Yajima, Koike, Yamasaki and Fujiwara[51] for various $[Co(en)_x(NH_3)_{6-2x-y}L_y]$ type complexes.

More precise estimations of chemical shifts have been tried by Juranic and his co-workers with consideration of lowering coordination symmetry[71-73] for the CoN_xO_{6-x} series. Au-Yeung and Eaton[93] extended the prediction of chemical shifts with trans-ligand pairs. Their estimation of chemical shifts and line width parameters of each ligand is consistent with the experimental and literature data. Their ligand parameters for chemical shift estimations express the "absolute chemical shift" namely that from the naked cobalt-59 nucleus. Although the uncertainty of absolute gyromagnetic ratio in the literature results in some abiguities, their estimation seems the most reasonable in covering the variety of chemical shifts of most octahedral cobalt(III) complexes. There must be some changes if a different gyromagnetic ratio is introduced, but it seems less important in the estimation of various cobalt complexes.

Nishizawa[59] tried to predict the cobalt-59 chemical shifts by cis-ligand pair parameters for various complexes, but there were severe deviations without the consideration of trans-pair parameters.

Another theoretical estimation was proposed by Bramley and his co-workers[113] with ligand field parameters. Their detailed study for twenty complexes of relatively high symmetry has elucidated the clear relationships between chemical shift and the spectrochemical parameter (Δ) and the Racah parameter (nephelauxetic ratio, β).

These theoretical explanations seem very interesting, but the generalization of such treatments to a wide range of mixed ligand complexes of lower symmetry is thought to be very hard and probably, the introduction of many other parameters will be necessary.

The estimation of the gyromagnetic ratio of the "naked" cobalt-59 nucleus, namely the origin of absolute chemical shift, has also been an important topic in the nuclear physics area. In the early stages of cobalt-NMR study, Walstedt, Wernick and Jaccarino[20] determined the gyromagnetic ratio 10.054 ± 0.02 MHz/T from the NMR of solid cobalt silicides. From solid cobalticenium nitrate, Spiess, Haas and Hartmann[26] obtained a very different value, 10.035 MHz/T.

By the extrapolation of the Griffith–Orgel plot of the $\lambda_{1\max}$ to zero (namely, Δ is infinitely large), the gyromagnetic ratio of the naked cobalt-59 nucleus can be estimated and the "absolute" gyromagnetic ratio of cobalt-59 can be determined. This estimation was carried out by Betteridge and Golding,[23] Fujiwara[24] and others. This extrapolated value from CoN_6 and CoO_6 complexes (10.015 MHz/T)[24] was nearly the same as those obtained from the single crystal study by Spiess.[26] Another estimation by Bramley[113] obtained the gyromagnetic ratio 10.048 MHz/T). However, wide-range extrapolation causes, inevitably, marked lowering of the precision of these estimations. Moreover, the estimated values from the complexes containing relatively soft ligand atoms such as phosphorus, sulfur and selenium do not coincide with the values obtained from the CoN_6, and CoO_6 series. The introduction of the exact nephelauxetic constants seems necessary.

Juranic[86,97] tried to estimate the gyromagnetic ratio of naked cobalt-59 with a different ligand grouping of higher symmetry, and obtained a value which is approximately equal to those obtained from solid cobalt silicides[20] by Walstedt rather than those reported by Spiess,[26] and much different from the values obtained using the normal Griffith–Orgel plot. From the consistency of the extrapolated value of each limited CoL_6 type complex, Juranic's gyromagnetic ratio seems more reasonable than the values customarily obtained from simple Griffith–Orgel plots.

4. EXPRESSION OF CHEMICAL SHIFT DATA

Customarily, the aqueous solution of potassium hexacyanocobaltate(III) has been recommended and widely used as a standard substance, and the high frequency side shift (low-field shift) is denoted as positive.[1-4] Several secondary standard substances have been proposed and used in many papers, for instance, tris(ethylenediamine)cobalt(III) cation, hexaamminecobalt(III) cation, and tris(acetylacetonato)cobalt(III) (in chloroform), because of the remarkably large distribution of chemical shifts among various complexes. Some authors used aqueous sodium hexanitrocobaltate(III), but there are some unclarified problems in the state of this complex species in aqueous solutions (see later), and it is therefore not recommended for use as a standard, although it has good water solubility and is readily obtained from many commercial sources.

The definition of chemical shifts containing the resonant frequency of a standard substance is as follows.

$$\sigma = (\gamma-\gamma_0)/\gamma_0 \text{ or } = (\nu-\nu_0)/\nu_0$$

However, many chemical shift measurements have been carried out at a constant frequency (field sweep) as noted above. In this case, chemical shifts are usually expressed as follows:

$$\sigma' = (\Delta H/H) = (H_s-H_0)/H_0 = (\gamma-\gamma_0)/\gamma$$

This σ' is not exactly equal to the above σ value, because the difference between the resonant frequencies of standard and sample cannot be neglected in nuclei in the large chemical shift range. This means that conversion of chemical shift data by simple addition–subtraction possibly causes too significant errors for detailed discussions.

There are almost 20 sets of chemical shift data for the hexaamminecobalt(III) complex, which seem to be divided into two groups, one has a value around 8100 ppm, and another 8170 ppm. The former data were obtained from field-sweep (constant frequency) measurements (σ'), and the latter from FT-NMR measurements or resonant frequency measurements (σ). This inconsistency disappears almost

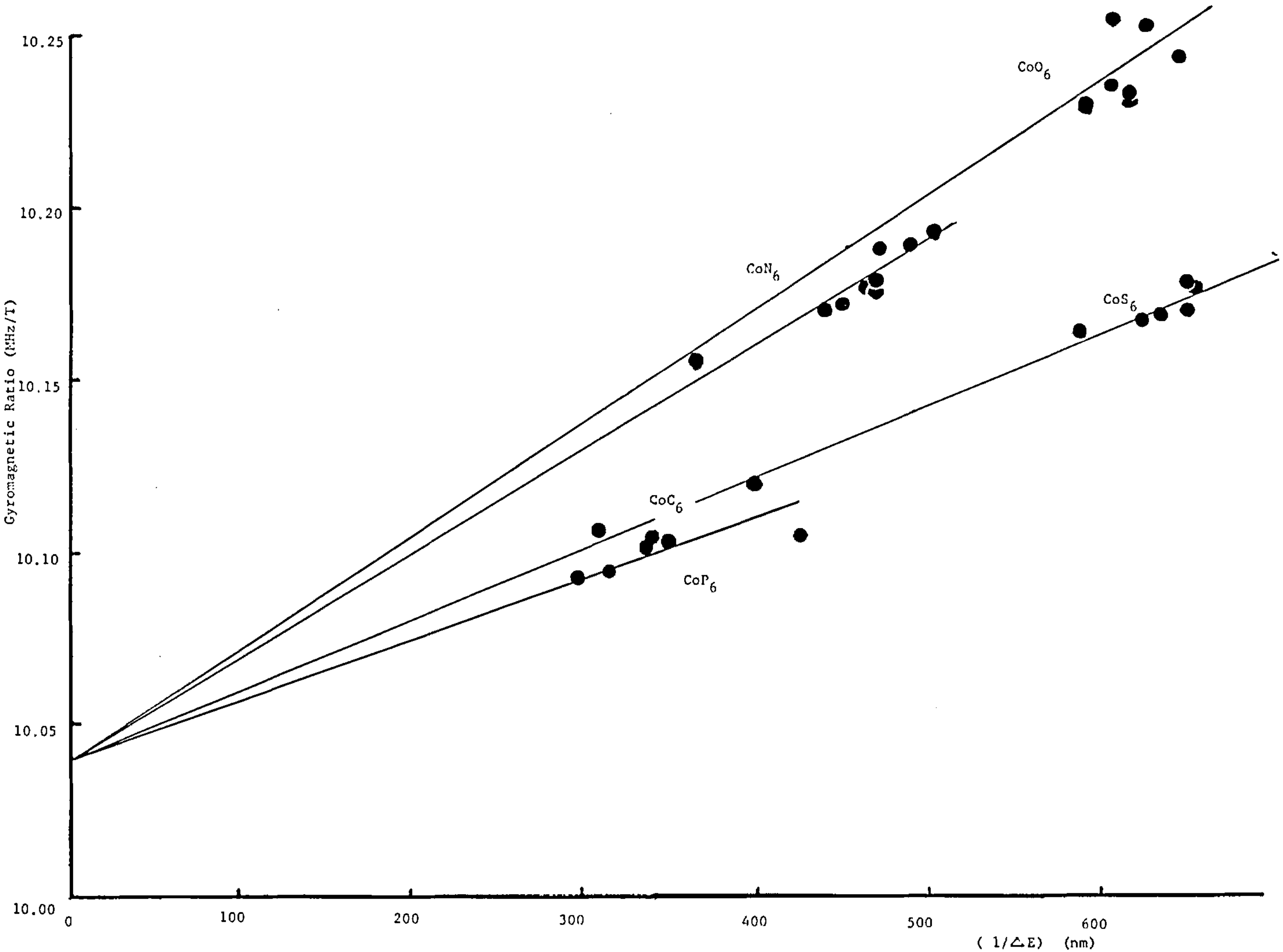


FIGURE 1 The Griffith–Orgel plot for typical cobalt(III) complexes of the CoL_6 type. Each linear line intercepts the gyromagnetic ratio axis at 10.04 (MHz/T), which is approximately equal to the value obtained by Juranic.[91]

perfectly with the conversion of σ' to σ. After this conversion, the mean value of the chemical shift is 8173 ppm with a standard deviation of 3 ppm. (With the exclusion of two extreme values, the standard deviation becomes only 1 ppm).

This consistency seems surprisingly good, because the chemical shift of cobalt(III) complexes is known to be dependent on temperature, pressure, and concentrations.

The chemical shift difference between hexacyanocobaltate(III) and tris(ethylenediamine)cobalt(III) is fairly large (7143 ppm), and it is necessary to select another secondary standard substance whose chemical shift situates around 3500 ppm. One of the candidates is *fac*-tricyanotriamminecobalt(III) (3314 ppm),[93] but its limited solubility and the difficulties of obtaining it from commercial sources have prevented its extended use. (The preparation of this complex is not as simple as for other popular complexes.)

The conversion of chemical shift data among the different standard substances is usually carried out by the addition–subtraction of chemical shift differences of each standard, as in the following

$$\sigma([\mathrm{Co(en)_3}]^{3+}) = \sigma([\mathrm{Co(CN)_6}]^{3-}) - 7145 \text{ (ppm)}$$
$$\sigma([\mathrm{Co(NH_3)_6}]^{3+}) = \sigma([\mathrm{Co(CN)_6}]^{3-}) - 8173 \text{ (ppm)}$$
$$\sigma([\mathrm{Co(acac)_3}]) = \sigma([\mathrm{Co(CN)_6}]^{3-}) - 12625 \text{ (ppm)}$$

If a more accurate conversion is needed, the above equations should be rewritten as follows, because the resonant conditions of the secondary standards cannot be assumed to be approximately equal to that of hexacyanocobaltate(III).

$$\sigma([\mathrm{Co(en)_3}]^{3+}) = \{\sigma([\mathrm{Co(CN)_6}]^{3-}) - 7145\}/1.007145 \text{ (ppm)}$$
$$\sigma([\mathrm{Co(NH_3)_6}]^{3+}) = \{\sigma([\mathrm{Co(CN)_6}]^{3-}) - 8173\}/1.008173 \text{ (ppm)}$$
$$\sigma([\mathrm{Co(acac)_3}]) = \{\sigma([\mathrm{Co(CN)_6}]^{3-}) - 12625\}/1.012625 \text{(ppm)}$$

The continuous-wave (CW) NMR spectral measurements have also been used throughout NMR history because the large difference of spectral line widths of cobalt-59 NMR is not necessarily favourable to FT measurements. Field-sweep measurements are usually applied to record the spectra in these CW measurements. The chemical shift data obtained from this field-sweep method should be different from the FT measurements, because the variation of chemical shift of cobalt-59 is much larger than for protons. Therefore, caution must be taken when comparing with other data.

The order of difference in many cobalt(III) complexes becomes one percent or less. In other words, the wide range distribution of chemical shift results in a significant bias from the difference of resonance condition of each standard substance. Moreover, recent pulsed Fourier-transform type NMR spectrometers can usually calculate the chemical shift value as the ratio of frequency difference against the frequency of pulse oscillators which is usually settled outside of the recording spectral range by built-in microcomputers. Therefore, machine-calculated chemical shift data on spectral charts cannot be directly accepted if detailed chemical shift data are necessary to the discussions.

To overcome these difficulties, a gyromagnetic ratio expression was recommended by Bramley and his groups.[113] This seems to be the revival of the first expression used by Proctor and Yu,[5] Freeman, Murray and Richards,[7] or Martin and White.[25] Modern NMR spectrometers have good stability of magnetic fields and resonant frequencies. The gyromagnetic ratios of hexacyanocobaltate(III) complex calculated from the different measurements seem consistent with each other (10.1058 ± 1 MHz/T), although they contain most of the earlier measurements (see Table 1). Therefore, it seems the most effective notations to eliminate the conversion errors. However, there are some significant deviations (or biases) in Bramley's data (10.1020), which might be attributed to instrumental origin, because their chemical shift data seem to be consistent with others obtained from independent origins. (The gyromagnetic ratio 10.1060 was obtained for hexacyanocobaltate(III) from our earlier measurements, but this is not accurate as we did not intend its use in this type of chemical shift expression.)

TABLE 1. Gyromagnetic ratio expression of several cobalt(III) complexes (often recommended as standard substances).

Complex	gyromagnetic ratio (MHz T^{-1})
$[Co(CN)_6]^{3-}$	10.1058 ± 1
$[Co(en)_3]^{3+}$	10.1779 ± 1
$[Co(NH_3)_6]^{3+}$	10.1883 ± 3
$[Co(acac)_3]/CDCl_3$	10.2338 ± 1
$[Co(C_2O_4)_3]^{3-}$	10.2371 ± 3

On the other hand, the accurate determination of only slight differences can be useful for medium effect studies, stereoisomers or isotopomer discrimination. For these purposes, the above "absolute" expression is unnecessary and inconvenient. The use of secondary standards would be a much better method. The complexes in Table 1 are recommended as the conventional secondary standards, which have relatively reproducible chemical shift (or gyromagnetic ratio) values in various different works.

5. LINE WIDTH

Earlier reports were mainly focussed on determining chemical shift data, and the spectrometers were not sufficient in obtaining reliable line-width data for the widely varying line widths. Therefore, impure samples occasionally caused erroneous assignments, because the coexistent species of narrower line widths are usually more easily determined than those of wider line widths especially by CW type spectrometers. Many cobalt(III) complexes are not easily purified without careful recrystallization or chromatographic separation, although the standard processes were summarized in the early decades of this century. The first collection of line-width data for cobalt-59 NMR was probably carried out by Hartmann and Sillescu.[11]

The NMR line widths of cobalt-59 can be affected by the following paragraphs, (i) dipolar relaxation, (ii) quadrupolar relaxation, (iii) broadening by scalar coupling, (iv) exchange reactions, and (v) chemical shift anisotropy.

Almost all low-spin type cobalt(III) complexes are so-called "substitution-inert", namely the ligand exchange rates for these complexes have a much smaller effect on NMR line shape than for any other metal complexes. Therefore, this ligand exchange contribution should be neglected in cobalt-59 NMR spectroscopy. Dipolar relaxation should be considered for samples in the solid state, but is not so important in the liquid states or when in solution.

Signal splitting by scalar coupling can be effective for complexes which have ligand atoms of non-zero spin, such as carbon-13, nitrogen-14,15, oxygen-17 and so on. However, these spin–spin couplings between cobalt-59 and these nuclei have been only rarely observed because of their low natural abundance or quadrupolar relaxation of the ligand nuclei which have lower symmetry and large field gradients, although several INDOR experiments revealed the existence of scalar couplings in relatively high symmetric complexes.[66]

Therefore, the most dominant factor of line-broadening of the diamagnetic cobalt-59 NMR spectra should be quadrupolar relaxation, and there is much experimental data to confirm this hypothesis. The quadrupolar relaxation is largely dependent on the electric field gradient at the central cobalt nucleus, which reflects mainly the symmetry of the ligand atom combination and configurations. Of course there are several exceptional cases which will be discussed later.

The quadrupolar relaxation rate, R_q, is expressed in the case of extreme narrowing with an axial electric field gradient (efg) as follows:

$$R_q = (3/40)\{(2I+3)/[I^2(2I-1)]\}(e^2Qq/h)\tau_E$$

where eQ is the nuclear quadrupole moment, τ_E is the reorientational correlation time for the electric field gradient (efg), and eq is the electric field gradient (efg) at the observed nucleus.

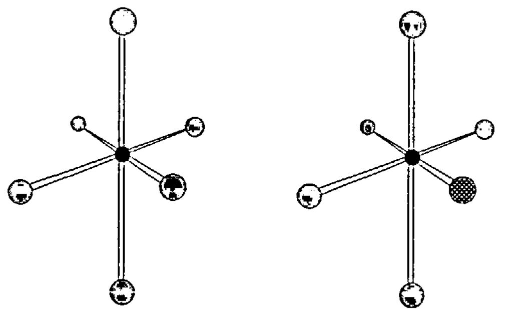
The magnitude of the electric field gradient at the cobalt-59 nucleus plays a dominant role in the determination of spectral shape. Simple point-charge or point-dipole model calculations give the wide variety of relative magnitudes of electric field gradients for binary mixed ligand complexes, which are shown in Figure 2. Facial CoA_3B_3 type complexes have a zero field gradient and the line widths for these complexes are usually much narrower than those of meridional isomers. These simple models were introduced by Yamasaki[22] for about 30 complexes for the first time, but it has been proved to be valid for a vast number of cobalt complexes of different classes since then. More detailed estimations were also carried out by Au-Yeung and Eaton[93] for $CoA_aB_bC_cD_d$-type complexes ($a + b + c + d = 6$).

The magnitude of efg seems largely dependent on the combination of ligand atoms and less on the ligand groups. The CoN_6 type complexes usually show smaller line widths than the other CoN_xL_{6-x} type complexes. Only the hydroxo–ammine–ethylenediamine mixed complexes showed relatively narrow spectra,[34,39] in spite of the ligand atom combination of CoN_xO_{6-x}.

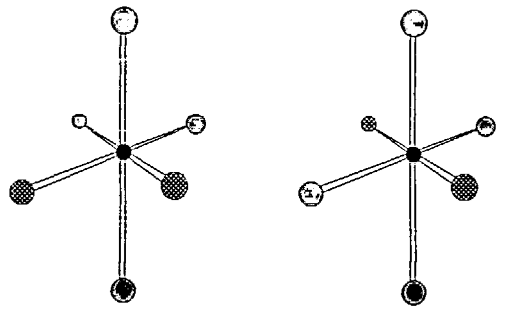
Of course there are some exceptional cases which show relatively large line widths in spite of higher ligand atom symmetry such as with CoP_6.[78,125] The larger line widths for these phosphite complexes can be attributed to the increase of electric field gradients from the distortion of the nearest configuration of ligand atoms by the repulsion between bulky groups attached on phosphorus atoms.

Some dioxygen complexes have been reported to show remarkable line width change with resonant field strengths.[93–95] This is an interesting and peculiar characteristic suggesting the existence of another mechanism determining the cobalt-59 relaxation rates.

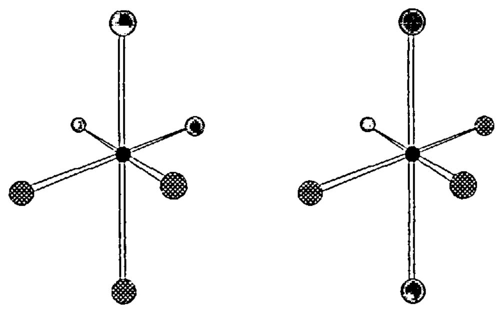
Chemical shift anisotropy has been the main interest of single crystal NMR study for several cobalt(III) complexes. The differences between σ_{zz} and σ_{xx}, σ_{yy} are of minor contribution to line widths in the relatively low-field NMR measurements. Spectral measurements with superconducting magnets revealed the importance of chemical shift anisotropy on the complexes of lower-symmetry.



CoA_6, CoB_6 CoA_5B, $CoAB_5$



cis-CoA_4B_2, *cis*-CoA_2B_4 *trans*-CoA_4B_2, *trans*-CoA_2B_4



fac-CoA_3B_3 *mer*-CoA_3B_3

FIGURE 2. The structure and relative electric field gradients (efg) of the typical binary complexes of the type CoA_xB_{6-x}.[22] The relative efg are estimated as follows:

CoA_6, CoB_6, *fac*-CoA_3B_3	0
CoA_5B, $CoAB_5$, *cis*-CoA_4B_2, *cis*-CoA_2B_4	2
mer-CoA_3B_3	3
trans-CoA_4B_2, *trans*-CoA_2B_4	4

For the CoA_xB_{6-x} series, the symmetric CoA_6 and CoB_6 type complexes and *facial* CoA_3B_3 type complexes show only weak field dependence on line width. A relatively large field dependence was observed in the case where the sites of two ligands were largely distant in the spectrochemical series. The line widths of *meridional*-tricyanotriamminecobalt(III) complex show remarkable field dependence, on the other hand, *facial*-tricyanotriammine(III) complex does not show a clear change even at 94 MHz.[95]

In the Table 1, the cobalt-59 chemical shift and line width data are summarized for typical complexes which were exactly expressed by gyromagnetic ratio. These complexes can be used as chemical shift standards. The spectral data for other complexes of cobalt(III) are shown in Table 2 according to the increase of chemical shift values (low-field shifts).

6. IDENTIFICATION OF ISOMERS

6.1. *Geometrical Isomer*

Geometrical isomers of the cobalt(III) complexes have been familiar from the early stages of coordination chemistry, and the difference in chemical shifts had been pointed out previously in the early stages of cobalt NMR,[7,8,22] for cis-trans isomeric pairs.

The cobalt-59 NMR line widths are clearly dependent on the quadrupolar relaxation as noted above. This quadrupolar relaxation rate reflects the electric field gradient at the central cobalt nucleus in these complexes. The electric field gradient can be estimated from the ligand atom configuration as shown above. From calculation using the point charge model, *facial* CoA_3B_3-type complexes would have zero electric field gradients, but the *meridional* CoA_3B_3 isomers would have non-zero field gradients. Moreover, the electric field gradient of the *trans* isomers of CoA_4B_2 type complexes should be much larger than those of the *cis* isomers.[22] (see Fig. 2).

Therefore, this rule holds almost all *cis-trans* isomer pair discriminations,[22] although there are a few exceptions such as $[Co(en)_2(OH)_2]^+$. Tarasov and his groups have studied the considerably large number of diethylenetriamine (dien) complexes of the type $Co(dien)X_3$ and the *mer-fac* isomer pairs showing analogous trends throughout their study.[101]

More general treatment of electric field gradient estimation for isomeric pairs was carried out by Au-Yeung and Eaton[93] from CoA_6 to $CoA_aB_bC_cD_d$ $(a+b+c+d=6)$ as cited above. Their estimated values are qualitatively so consistent with much of the reported data as to discriminate isomeric pairs, but there are some inconsistencies which should be precisely re-examined by modern instruments with more reliable samples than used in these early studies.

6.2 *Linkage Isomer*

It has been long known that there are many linkage isomer pairs in cobalt(III) complexes, such as nitrito–nitro, or thiocyanato–isothiocyanato complexes. The identification of these isomer pairs can be easily accomplished by cobalt-59 NMR as well as infrared spectroscopy. The earliest trial to discriminate between these isomer pairs by cobalt-59 NMR was carried out in 1967.[19] The differences in the ligand atom configuration are usually concluded from the chemical shift and line-width data.[93,101]

TABLE 2a. Gyromagnetic ratios of cobalt(III) complexes

Complex	Gamma(Co)	σ(I)	Lit. No.
$[Co(CN)_6]^{3-}$	10.1020	0	113
$[Co(CN)_6]^{3-}$	10.1037	0	5
$[Co(diars)_3]^{3+}$	10.1050	−100	97
$[Co(CN)_6]^{3-}$	10.1057	0	25
$[Co(CN)_6]^{3-}$	10.1057	0	7
$[Co(CN)_6]^{3-}$	10.1060	0	86
$[Co(CNO)_6]^{3-}$	10.1190	1300	97
$[Co(NH_3)_3(CN)_3]$, *mer-*	10.1356	3326	113
$[Co(NH_3)_4(CN)_2]^+$, *cis-*	10.1530	5049	113
$[Co(dmgH)_3]^{3+}$	10.1550	4880	97
$[Co(triarsine)_2]^{3+}$, (*)	10.1552	4902	25
$[Co(triarsine)_2]^{3+}$, (*)	10.1602	5398	25
$[Co(S_2CBz)_3]$	10.1650	5830	97
$[Co(S_2COEt)_3]$	10.1658	6316	113
$[Co(tacn)_2]^{3+}$	10.1666	6394	113
$[Co(S_2COEt)_3]$	10.1684	6208	25
$[Co(S_2COMe)_3]$	10.1690	6250	97
$[Co(S_2COEt)_3]$	10.1690	6234	86
$[Co(S_2CO(i\text{-}Pr))_3]$	10.1695	6319	25
$[Co(NH_3)_5CN]^{2+}$	10.1695	6681	113
$[Co(S_2CS)_3]^{3-}$	10.1700	6390	97
$[Co(S_2CN(Me)_2)_3]$	10.1734	6704	25
$[Co(Se_2CN(Me)_2)_3]$	10.1739	6759	25
$[Co(en)_3]^{3+}$	10.1742	7147	113
$[Co(NH_3)_2(NO_2)_4]^-$, *trans-*	10.1759	6950	7
$[Co(tame)_2]^{3+}$	10.1770	7424	113
$[Co(S_2C\text{-}(pyrr))_3]$	10.1772	7074	25
$[Co(en)_3]^{3+}$	10.1774	7300	5
$[Co(en)_2Cl_2]^+$, *trans-* (*)	10.1775	7109	7
$[Co(en)_2CO_3]^+$ (*)	10.1778	7131	7
$[Co(en)_3]^{3+}$	10.1779	7144	25
$[Co(en)_3]^{3+}$	10.1780	7124	86
$[Co(en)_3]^{3+}$	10.1782	7177	7
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-*	10.1784	7199	7
$[Co(NO_2)_6]^{3-}$ (**)	10.1785	7400	5
$[Co(pn)_3]^{3+}$(isomer mixture)	10.1787	7220	7
$[Co(S_2CNH_2)_3]$	10.1788	7231	25
$[Co(S_2CNH_2)_3]$	10.1790	7223	86
$[Co(NH_3)_4(NO_2)_2]^+$, *cis-*	10.1794	7290	7
$[Co(NO_2)_6]^{3-}$ (**)	10.1809	7444	25
$[Co(NO_2)_6]^{3-}$ (**)	10.1814	7490	7
$[Co(NH_3)_5(S_2O_3)]^+$	10.1840	8117	113
$[Co(NH_3)_5SCN]^{2+}$	10.1846	8177	113
$[Co(NH_3)_6]^{3+}$	10.1849	8206	113
$[Co(NO_2)_6]^{3-}$ (**)	10.1855	8100	5
$[Co(NH_3)_5NCS]^{2+}$	10.1863	8345	113
$[Co(NO_2)_6]^{3-}$ (**)	10.1871	8060	7
$[Co(NH_3)_5NH_2OSO_2]^{2+}$	10.1873	8444	113
$[Co(NH_3)_6]^{3+}$	10.1875	8300	5
$[Co(NH_3)_6]^{3+}$	10.1880	8114	86
$[Co(NH_3)_6]^{3+}$	10.1883	8175	25

TABLE 2a (*continued*)

Complex	Gamma(Co)	σ(1)	Lit. No.
$[Co(NH_3)_6]^{3+}$	10.1887	8218	7
$[Co(NH_3)_5(N_3)]^{2})$	10.1897	8681	113
$[Co(tn)_3]^{3+}$	10.1900	8312	86
$[Co(en)_2(C_2O_4)]^+$	10.1902	8731	113
$[Co(NH_3)_5I]^{2+}$	10.1914	8849	113
$[Co(en)_2(mal)]^+$	10.1916	8870	113
$[Co(NH_3)_5Cl]^{2+}$	10.1918	8889	113
$[Co(NH_3)_5Br]^{2+}$	10.1921	8919	113
$[Co(bn)_3]^{3+}$	10.1930	8670	97
$[Co(S_2P(OEt)_2)_3]$	10.1934	9048	113
$[Co(NH_3)_5(O_2C(Me))]^{2+}$	10.1940	9107	113
$[Co(NH_3)_5(OH_2)]^{3+}$	10.1944	9147	113
$[Co(NH_3)_5(OH)]^{2+}$	10.1949	9196	113
$[Co(S_2P(OEt)_2)_3]$	10.1964	8978	25
$[Co(NH_3)_5NO_2]^{2+}$	10.1972	9423	113
$[Co(NH_3)_4CO_3]^+$	10.1981	9146	7
$[Co(NH_3)_5F]^{2+}$	10.2000	9701	113
$[Co(NH_3)_4CO_3]^+$	10.2041	9734	7
$[Co(en)(C_2O_4)_2]^-$	10.2088	10572	113
$[Co(en)(mal)_2]^-$	10.2119	10879	113
$[Co(Mo_6O_{24}H_6]^{3-}$	10.2288	12551	113
$[Co(acac)_3]/CHCl_3$	10.2322	12520	25
$[Co(C_2O_4)_3]^{3-}$	10.2332	12987	113
$[Co(acac)_3]/C_6H_6$	10.2338	12680	7
$[Co(C_2O_4)_3]^{3-}$	10.2350	13000	5
$[Co(C_2O_4)_3]^{3-}$	10.2368	12976	25
$[Co(C_2O_4)_3]^{3-}$	10.2370	12963	86
$[Co(C_2O_4)_3]^{3-}$	10.2375	13040	7
$[Co(mal)_3]^{3-}$	10.2436	14017	113
$[Co(CO_3)_3]^{3-}$	10.2485	14130	7
$[Co(OH_2)_6]^{3+}$	10.2540	15047	113

TABLE 2b. Chemical shift measured from hexacyanocobaltate(III), σ(1), and line width data.

Complex	σ(1)	Width (Hz)	Lit. No.
$[Co(en)_2Cl_2]^+$, *cis*- (1M HCl)		5100	11
$[Co(en)_2Cl_2]^+$, *trans*-		7800	11
$[Co(NH_3)_3](OH)_2(\mu\text{-}C_4H_2O_2CO(NH_3)_5)]^{5+}$	undetectable		56
$[Co(diphos)_3]^{3+}$	−2600	9000	118
$[Co(Me_2PCH_2CH_2PMe_2)_3]^{3+}$	−2530	10000	118
$[Co(C_5H_5)_2]^+$	−2200		26
$[Co(o\text{-}C_6H_4(PPh_2)_2)_3]^{3+}$	−2120	11000	118
$[Co(P(OCH_2)_3CMe]_6]^{3+}$	−1243	75	78
$[Co(P(OMe)(OCH_2CH_2O))_6]^{3+}$	−1185	2500	78
$[Co(o\text{-}C_6H_4(PMe_2)(AsMe_2))_3]^{3+}$	−910	14000	118
$[Co(diars)_3]^{3+}$	−520	6000	118
$[Co(P(OMe)(OCHMeCH_2CHMeO))_6]^{3+}$	−356	3000	78
$[Co(diars)_3]^{3+}/DMSO$	−320		118
$[Co(P(OMe)(OCHMeCH_2CHMeO))_6]^{3+}$	−307	3000	78

TABLE 2b (*continued*)

Complex	$\sigma(1)$	Width (Hz)	Lit. No.
$[Co(P(OMe)_3)_6]^{3+}$	−305	150	78
$[Co(P(OMe)_3)_6]^{3+}$	−304	340	61
$[Co(diars)_3]^{3+}$	−100		97
$[Co(CN)_6]^{3-}$	0	50	22
$[Co(CN)_6]^{3-}$	0	5	95
$[Co(CN)_6]^{3-}$	0	0	95
$[Co(CN)_6]^{3-}$	0		113
$[Co(CN)_6]^{3-}$	0		11
$[Co(CN)_6]^{3-}$	0		12
$[Co(CN)_6]^{3-}$	0		8
$[Co(CN)_6]^{3-}$	0		65
$[Co(CN)_6]^{3-}$	0	50	10
$[Co(CN)_6]^{3-}$	0	5	93
$[Co(CN)_6]^{3-}$	0		25
$[Co(CN)_6]^{3-}$	0	5	95
$[Co(CN)_6]^{3-}$	0	175	29
$[Co(CN)_6]^{3-}$	0		7
$[Co(CN)_6]^{3-}$	0		86
$[Co(CN)_6]^{3-}$	0		5
$[Co(CN)_6]^{3-}$ $-\{^{13}C\}$	0.851		13
$[Co(CN)_6]^{3-}$ $-\{^{13}C\}$	0.914		12
$[Co(CN)_6]^{3-}$ $-\{^{15}N\}_6$	1.18		12
$[Co(CN)_6]^{3-}$ $-\{^{13}C\}_2$	1.709		13
$[Co(CN)_6]^{3-}$ $-\{^{13}C\}_2$	1.832		12
$[Co(CN)_6]^{3-}$ $-\{^{13}C\}_3$	2.56		13
$[Co(CN)_6]^{3-}$ $-\{^{13}C\}_3$	2.743		12
$[Co(CN)_6]^{3-}$ $-\{^{13}C\}_4$	3.659		12
$[Co(CN)_6]^{3-}$ $-\{^{13}C\}_5$	4.58		12
$[Co(CN)_6]^{3-}$ $-\{^{13}C\}_6$	5.463		12
$[Co(o\text{-}C_6H_4(PMe_2)(SbMe_2))_3]^{3+}$	390		124
$[Co(CN)_5NO_2]^{3-}$	598	4200	95
$[Co(CN)_5NO_2]^{3-}$	599	5100	95
$[Co(CN)_5NO_2]^{3-}$	619	3767	95
$[Co(CN)_5I]^{3-}$	780	9970	27
$[Co(CN)_5NH_3]^{2-}$	1162	3131	95
$[Co(CN)_5NH_3]^{2-}$	1168	3131	93
$[Co(CN)_5NH_3]^{2-}$	1169	4470	95
$[Co(CN)_5NH_3]^{2-}$	1174	3747	95
$[Co(CN)_5Br]^{3-}$	1220	11370	27
$[Co(CNO)_6]^{3-}$	1300		97
$[Co(CN)_5NO_2]^{3-}$	1400	10000	22
$[Co(Me_2PCH_2CH_2PMe_2)_2Cl_2]^+$, *trans-*	1660	14000	118
$[Co(diphos)_2Cl_2]^+$, *trans-*	1710	16500	118
$[Co(o\text{-}C_6F_4(PMe_2)_2)_2Cl_2]^+$, *trans-*	1740	14000	118
$[Co(CN)_5(OH_2)]^{2-}$	1822	6120	27
$[Co(CN)_5(OH)]^{3-}$	1840	5250	27
$[Co(en)(CN)_4]^-$	1998	5479	95
$[Co(en)(CN)_4]^-$, *cis-*	2006	5410	93
$[Co(en)(CN)_4]^-$	2006	5438	95
$[Co(en)(CN)_4]^-$	2013	5410	95
$[Co(PhP(CH_2CH_2PPh_2)_2Cl_3]$	2100	16000	118

TABLE 2b (*continued*)

Complex		σ(1)	Width (Hz)	Lit. No.
$[\mathrm{Co}(o\text{-}\mathrm{C_6H_4(PPh_2)_2)_2Cl_2}]^+$, *trans-*		2220	15000	118
$[\mathrm{Co(Ph_2PCH{=}CHPPh_2)_2Cl_2}]^+$, *trans-*		2250	20000	118
$[\mathrm{Co(P(CH_2CH_2PPh_2)_3)Cl_2}]^+$, *cis-*		2360	16000	118
$[\mathrm{Co(PhP(CH_2CH_2PPh_2)_2Br_3}]$		2430	16000	118
$[\mathrm{Co(NH_3)_2)(CN)_4}]^-$, *cis-*		2457	2673	93
$[\mathrm{Co}(o\text{-}\mathrm{C_6H_4(PMe_2)(AsMe_2))_2Cl_2}]^+$, *trans-*		2490	19500	118
$[\mathrm{Co}(o\text{-}\mathrm{C_6H_4(PPh_2)(SMe))_3}]^{3+}$		2620		124
$[\mathrm{Co(NH_3)_2(CN)_4}]^-$, *trans-*		2744	13096	93
$[\mathrm{Co}(o\text{-}\mathrm{C_6H_4(PPh)_2)_2Br_2}]^+$, *trans-*		2750	14000	118
$[\mathrm{Co(As(CH_2CH_2CH_2AsMe_2)_3)Cl_2}]^+$, *cis-*		2820	14500	118
$[\mathrm{Co(Me_2PCH_2CH_2PMe_2)_2I_2}]^+$, *trans-*		2830	13000	118
$[\mathrm{Co(diars)_2Cl_2}]^+$, *trans-*		2830	15000	118
$[\mathrm{Co(diars)_2Cl_2}]^+$, *cis-*		2860	12000	118
$[\mathrm{Co(diars)_2Br_2}]^+$, *trans-*		2880	14000	118
$[\mathrm{Co(dmgH)_2(py)(SnPh_3)}]$		3090		45
$[\mathrm{Co(dmgH)_2(ba)(SnPh_3)}]$		3150		45
$[\mathrm{Co(NH_3)_3(CN)_3}]$, *fac-*	(59.035 MHz)	3312	720	95
$[\mathrm{Co(NH_3)_3(CN)_3}]$, *fac-*	(94.457 MHz)	3313	750	95
$[\mathrm{Co(NH_3)_3(CN)_3}]$, *fac-*	(21.252 MHz)	3314	618	93
$[\mathrm{Co(NH_3)_3(CN)_3}]$, *fac-*	(21.252 MHz)	3317	618	95
$[\mathrm{Co(dmgH)_2Me(NH_2Bz)}]$		3320		45
$[\mathrm{Co(NH_3)_3(CN)_3}]$, *mer-*		3326		113
$[\mathrm{Co(dmgH)_2(Me)(NC_5H_5)}]$		3370		45
$[\mathrm{Co(dmgH)_2(CN(c\text{-}Hex))I}]$		3400		85
$[\mathrm{Co(dmgH)_2(CN(c\text{-}Hex))_2}]^+$		3410		85
$[\mathrm{Co(dmgH)_2(Bu)(NC_5H_5)}]$		3420		45
$[\mathrm{Co}(o\text{-}\mathrm{C_6H_4(PPh_2)(SMe))_2Br_2}]^+$		3430		124
$[\mathrm{Co}(o\text{-}\mathrm{C_6H_4(PPh_2)(SMe))_2Cl_2}]^+$		3475		124
$[\mathrm{Co(NH_3)_4(CN)_2}]^+$, *trans-*	(21.252 MHz)	3498	14810	93
$[\mathrm{Co(dmgH)_2(CN(c\text{-}Hex))Br}]$		3500		85
$[\mathrm{Co(dmgH)_2(CN(c\text{-}Hex))Cl}]$		3600		85
$[\mathrm{Co(dmgH)_2(CN(c\text{-}Hex))(NO_2)}]$		3690		85
$[\mathrm{Co(NH_3)_3(CN)_3}]$, *mer-*	(95.457 MHz)	3947	14078	95
$[\mathrm{Co(NH_3)_3(CN)_3}]$, *mer-*	(59.035 MHz)	3976	10808	95
$[\mathrm{Co(NH_3)_3(CN)_3}]$, *mer-*	(21.252 MHz)	3991	4542	95
$[\mathrm{Co(NH_3)_3(CN)_3}]$, *mer-*	(21.252 MHz)	3991	4542	93
$[\mathrm{Co(dmgH)_2(Me)(OH_2)}]$		4020		45
$[\mathrm{Co}(o\text{-}\mathrm{C_6H_4(PMe_2)(SbMe_2))_2Br_2}]^+$		4280		124
$[\mathrm{Co}(o\text{-}\mathrm{C_6H_4(PMe_2)(SbMe))_2Cl_2}]^+$		4330		124
$[\mathrm{Co(en)_2(CN)_2}]^+$, *cis-*	(94.457 MHz)	4364	5513	95
$[\mathrm{Co(diars)_2I_2}]^+$, *trans-*		4370	15000	118
$[\mathrm{Co(en)_2(CN)_2}]^+$, *cis-*	(21.252 MHz)	4379	3700	93
$[\mathrm{Co(en)_2(CN)_2}]^+$, *cis-*	(21.252 MHz)	4384	3700	95
$[\mathrm{Co(en)_2(CN)_2}]^+$, *cis-*	(59.035 MHz)	4388	5408	95
$[\mathrm{Co}(o\text{-}\mathrm{C_6H_4(PPh_2)(SeMe))_2Br_2}]^+$		4400		124
$[\mathrm{Co}(o\text{-}\mathrm{C_6H_4(PPh_2)(SeMe))_2Cl_2}]^+$		4445		124
$[\mathrm{Co(Me_2SbCH_2CH_2CH_2SbMe_2)_2Br_2}]^+$		4450		124
$[\mathrm{Co}(o\text{-}\mathrm{C_6H_4(SbMe_2)_2)_2Cl_2}]^\bullet$		4575		124
$[\mathrm{Co(dmgH)_2(NCMe)I}]$		4620		85
$[\mathrm{Co}(o\text{-}\mathrm{C_6H_4(SbMe_2)_2)_2Br_2}]^+$		4710		124
$[\mathrm{Co(en)_2(CN)_2}]^+$, *trans-*	(59.035 MHz)	4718	12025	95

TABLE 2b (*continued*)

Complex		$\sigma(1)$	Width (Hz)	Lit. No.
$[Co(en)_2(CN)_2]^+$, *trans*-	(94.45 MHz)	4726	16690	95
$[Co(en)_2(CN)_2]^+$, *trans*-	(21.252 MHz)	4727	8089	93
$[Co(en)_2(CN)_2]^+$, *trans*-	(21.252 MHz)	4736	8089	95
$[Co(dmgH)_3]^{3+}$		4880		97
$[Co(triarsine)_2]^{3+}$(*)		4902		25
$[Co(NH_3)_4(CN)_2]^+$, *cis*-		5049		113
$[Co(dmgH)_2(NH_3)_2]^+$		5120		45
$[Co(NH_3)_4(CN)_2]^+$, *cis*-	(21.252 MHz)	5132	2489	93
$[Co(NH_3)_4(CN)_2]^+$, *cis*-	(21.252 MHz)	5132	2489	95
$[Co(NH_3)_4(CN)_2]^+$, *cis*-	(59.035 MHz)	5164	7059	95
$[Co(NH_3)_4(CN)_2]^+$, *cis*-	(94.457 MHz)	5173	9656	95
$[Co(dmgH)_2(NH_3)_2]^{3+}$	(59.035 MHz)	5370	7299	95
$[Co(dmgH)_2(NH_3)_2]^{3+}$	(94.457 MHz)	5382	9189	95
$[Co(dmgH)_2(NH_3)_2]^{3+}$	(21.252 MHz)	5386	6123	95
$[Co(triarsine)_2]^{3+}$ (*)		5398		25
$[Co(o\text{-}C_6H_4(PMe_2)(SbMe_2))_2I_2]^+$		5480		124
$[Co(bimp)_2(NH_3)_2]^+$		5510		45
$[Co_2(S_2CN(c\text{-}Hex)_2)_5]^+$ (II)		5570		112
$[Co_2(S_2C\text{-}(2,6\text{-}Me_2pip))_5]^+$ (II)		5790		112
$[Co(S_2CBz)_3]$		5830		97
$[Co_2(S_2C\text{-}(2\text{-}Mepip))_5]^+$ (II)		5890		112
$[Co(NH_3)_4(CN)(SO_3)]$		5910		32
$[Co_2(S_2C\text{-}(pip))_5]^+$ (II)		5960		112
$[Co_2(S_2CN(Bz)_2)_5]^+$ (II)		5960		112
$[Co_2(S_2CN(Pr)_2)_5]^+$ (II)		5970		112
$[Co_2(S_2C\text{-}(4\text{-}Mepip))_5]^+$ (II)		5970		112
$[Co_2(S_2CN(Et)_2)_5]^+$ (II)		5980		112
$[Co(S_2CN(Bu)(t\text{-}Bu))_3]/CH_2Cl_2$		5990	1510	111
$[Co_2(S_2C\text{-}(morph))_5]^+$ (II)		5990		112
$[Co(NH_3)_5SO_3]^{2+}$		6030	430	11
$[Co_2(S_2CN(Me)_2)_5]^+$ (II)		6050		112
$[Co(S_2COEt)_3]$		6100		17
$[Co(NH_3)NO_2)_5]^{2-}$		6100		82
$[Co_2(S_2CN(c\text{-}Hex)_2)_5]^+$ (I)		6200		112
$[Co(S_2COEt)_3]$		6208		25
$[Co(NH_3)_2(NO_2)_4]^-$		6220		82
$[Co(S_2COEt)_3]$		6234		86
$[Co(S_2COMe)_3]$		6250		97
$[Co(Se_2CN(c\text{-}Hex)_2)_3]$		6260		115
$[Co_2(S_2C\text{-}(pyrr))_5]^+$ (II)		6260		112
$[Co(S_2COEt)_3]$		6316		113
$[Co(S_2COCH(Me)_2)_3]$		6319		25
$[Co(en)_2(NO_2)_2]^+$, *trans*-	(94.457 MHz)	6319	1579	95
$[Co(en)_2(NO_2)_2]^+$, *trans*- $/H_2O$	(94.457 MHz)	6319	1579	96
$[Co(en)_2(NO_2)_2]^+$, *trans*, $/H_2O$	(21.252 MHz)	6323	1366	96
$[Co(en)_2(NO_2)_2]^+$, *trans*	(21.252 MHz)	6323	1366	95
$[Co(en)_2(NO_2)_2]^+$, *trans*,	(59.035 MHz)	6329	1430	95
$[Co(en)_2(NO_2)_2]^+$, *trans*- $/H_2O$	(59.035 MHz)	6329	1430	96
$[Co(S_2CN(c\text{-}Hex)_2)_3]$		6330	1890	111
$[Co(S_2CN(c\text{-}Hex)_2)_3]$		6330		115
$[Co(S_2CN(c\text{-}Hex)_2)_3]$		6330		112

TABLE 2b (*continued*)

Complex		$\sigma(1)$	Width (Hz)	Lit. No.
$[Co(S_2CN(s\text{-}Bu)_2)_3]$ /CH_2Cl_2		6350	1500	111
$[Co(en)_2(NO_2)_2]^+$, *trans-*		6350		8
$[Co(Se_2CN)i\text{-}Pr)_2)_3]$		6360		115
$[Co(S_2CO(i\text{-}Pr)_2)_3]$		6360	300	22
$[Co(S_2CN(i\text{-}Pr)(c\text{-}Hex))_3]$		6360	1700	111
$[Co(S_2COEt)_3]$		6360	500	22
$[Co(en)_2(NO_2)_2]^+$, *trans-* /MeCN	(21.252 MHz)	6361	155	96
$[Co(en)_2(NO_2)_2]^+$, *trans-* /MeCN	(94.457 MHz)	6366	240	96
$[Co(en)_2(NO_2)_2]^+$, *trans-* /MeCN	(59.035 MHz)	6372	163	96
$[Co(en)_2(NO_2)_2]^+$, *trans-* /MeOH	(21.252 MHz)	6374	716	96
$[Co(en)_2(NO_2)_2]^+$, *trans-* /MeOH	(94.457 MHz)	6383	800	96
$[Co(en)_2(NO_2)_2]^+$, *trans-* /DMSO	(21.252 MHz)	6387	3963	96
$[Co(en)_2(NO_2)_2]^+$, *trans-* /MeOH	(59.035 MHz)	6387	751	96
$[Co(S_2CN(i\text{-}Pr)_2)_3]$ /CH_2Cl_2		6390	1030	111
$[Co(S_2CS)_3]^{3-}$		6390		97
$[Co(S_2CN(i\text{-}Pr)_2)_3]$		6390		115
$[Co(tacn)_2]^{3+}$		6394		113
$[Co(dien)(NO_2)_3]$, *mer-* /H_2O	(21.252 MHz)	6394	1620	96
$[Co(en)_2(NO_2)_2]^+$, *trans-* /DMSO	(94.457 MHz)	6396	4400	96
$[Co(dien)(NO_2)_3]$, *mer-* /H_2O	(59.035 MHz)	6397	2127	96
$[Co(dien)(NO_2)_3]$, *mer-* /H_2O	(94.457 MHz)	6399	3204	96
$[Co_2(S_2C\text{-}(2,6\text{-}Me_2pip))_5]^+$ (I)		6400		112
$[Co(en)_2(NO_2)_2]^+$, *trans-* /DMSO	(59.035 MHz)	6401	3642	96
$[Co(dien)(NO_2)_3]$, *mer-* /MeOH	(21.252 MHz)	6418	1826	96
$[Co(S_2CN(Hex)_2)(S_2CN(c\text{-}Hex)_2)_2]$		6420		111
$[Co(dien)(NO_2)_3]$, *mer-* /MeCN	(21.252 MHz)	6425	610	96
$[Co(dien)(NO_2)_3]$, *mer-* /MeOH	(59.035 MHz)	6428	1969	96
$[Co(dien)(NO_2)_3]$, *mer-* /MeOH	(94.457 MHz)	6431	2400	96
$[Co(dien)(NO_2)_3]$, *mer-* /MeCN	(94.457 MHz)	6435	1000	96
$[Co(dien)(NO_2)_3]$, *mer-* /Me_2CO	(21.252 MHz)	6435	956	96
$[Co(dien)(NO_2)_3]$, *mer-* /Me_2CO	(59.035 MHz)	6439	926	96
$[Co(S_2C\text{-}(pip)(S_2CN(c\text{-}Hex)_2)_2]$		6440		111
$[Co(dien)(NO_2)_3]$, *mer-* /Me_2CO	(94.457 MHz)	6449	1000	96
$[Co(S_2CN(Et)_2)_3]$		6450	300	22
$[Co(S_2CN)Bu)_2)(S_2CN(c\text{-}Hex)_2)_2]$		6450		111
$[Co(dien)(NO_2)_3]$, *mer-* /MeCN	(59.035 MHz)	6451	857	96
$[Co(S_2CSEt)_3]$		6460		17
$[Co(dien)(NO_2)_3]$, *mer-* /DMSO	(94.457 MHz)	6463	7130	96
$[Co(en)_2(NO_2)_2]^+$, *cis-*		6470		8
$[Co(S_2CN(Et)_2)(S_2CN(c\text{-}Hex)_2)_2]$		6470		111
$[Co(NH_3)_3(NO_2)_3]$		6470		82
$[Co(dien)(NO_2)_3]$, *mer-* /DMSO	(21.252 MHz)	6471	3853	96
$[Co(dien)(NO_2)_3]$, *mer-* /DMSO	(59.035 MHz)	6476	5491	96
$[Co(NH_2OH)_6]^{3+}$		6500	210	22
$[Co(en)_2(NO_2)_2]^+$, *trans-*		6500		26
$[Co(S_2CN(Bu)_2)(S_2CN(i\text{-}Pr)_2)_2]$		6520		111
$[Co(S_2CN(Hex)_2)(S_2CN(i\text{-}Pr)_2)_2]$		6530		111
$[Co(S_2C\text{-}(morph))(S_2CN(i\text{-}Pr)_2)_2]$		6530		111
$[Co(S_2CN(Oct)_2)(S_2CN(i\text{-}Pr)_2)_2]$		6530		111
$[Co(S_2CN(Et)_2)(S_2CN(i\text{-}Pr)_2)_2]$		6530		111

TABLE 2b (*continued*)

Complex		σ(I)	Width (Hz)	Lit. No.
Co(S$_2$CN(Bz)$_2$)$_5$]$^+$ (I)		6540		112
[Co(S$_2$CN(Me)$_2$)(S$_2$CN(*i*-Pr)$_2$)$_2$]		6540		111
[Co(S$_2$C-(2,6-Me$_2$pip))$_3$]		6540	1300	111
[Co(S$_2$C-(2,6-Me$_2$pip))$_3$]		6540		112
[Co(S$_2$C-(2-Mepip))$_5$]$^+$ (I)		6550		112
[Co(S$_2$C-(morph)(S$_2$CN(c-Hex)$_2$)$_2$]		6550		111
[Co(amben)(^{15}NO)] /CD$_2$Cl$_2$ (I)		6559	4800	121
[Co(*o*-C$_6$H$_4$(SbMe$_2$)$_2$)$_2$I$_2$]$^+$		6560		124
[Co(Me$_2$SbCH$_2$CH$_2$CH$_2$SbMe$_2$)$_2$I$_2$]$^+$		6565		124
[Co(en)$_2$(NO$_2$)$_2$]$^+$, *trans-*		6570	640	11
[Co(NH$_3$)$_5$CN]$^{2+}$		6570		32
[Co(S$_2$CN(Me)$_2$)(S$_2$CN(c-Hex)$_2$)$_2$]		6570		111
[Co(S$_2$C-(pyrr))(S$_2$CN(c-Hex)$_2$)$_2$]		6590		111
[Co(S$_2$CN(Hex)$_2$)$_2$(S$_2$CN(c-Hex)$_2$)]		6600		111
[Co(S$_2$C(pip))$_2$(S$_2$CN(c-Hex)$_2$)]		6610		111
[Co(S$_2$CN(Bu)$_2$)$_2$(S$_2$CN(c-Hex)$_2$)]		6610		111
[Co$_2$(S$_2$C-(pip))$_5$]$^+$ (I)		6620		112
[Co(bipy)$_3$]$^{3+}$		6620		8
[Co(NH$_2$OH)$_6$]$^{3+}$		6624		68
[Co(S$_2$CN(Et)$_2$)$_2$(S$_2$CN(c-Hex)$_2$)]		6630		111
[Co(S$_2$CN(Bu)$_2$)$_2$(S$_2$CN(*i*-Pr)$_2$)]		6630		111
[Co$_2$(S$_2$CN(Pr)$_2$)$_5$]$^+$ (I)		6630		112
[Co(S$_2$CN(Et))$_3$]		6630		17
[Co(S$_2$CN(*i*-Bu)$_2$)$_3$]		6640		115
[Co$_2$(S$_2$C-(4-Mepip))$_5$]$^+$ (I)		6640		112
[Co(S$_2$CN(*i*-Bu)$_2$)$_3$] /CH$_2$Cl$_2$		6640	1630	111
[Co(NH$_3$)$_5$CN]$^{2+}$	(21.252 MHz)	6641	3260	94
[Co(S$_2$CN(Et)$_2$(^{15}NO)] /CDCl$_3$		6642	1150	121
[Co(NH$_3$)$_5$CN]$^{2+}$	(94.457 MHz)	6645	14385	94
[Co(NH$_3$)$_5$CN]$^{2+}$	(59.035 MHz)	6646	8662	94
[Co(S$_2$CN(Bz)$_2$)$_3$]		6650	2400	111
[Co(S$_2$CN(Pr)(Ph))$_3$]		6650	2000	111
[Co(inaa)$_3$]		6650		19
[Co(S$_2$CN(Bz)$_2$)$_3$]		6650		112
[Co(S$_2$C-(pyrr))(S$_2$CN(*i*-Pr)$_2$)$_2$]		6650		111
[Co(S$_2$CN(Me)(Ph))$_3$] /CHCl$_3$		6660	1150	111
[Co(S$_2$C-(morph))$_2$(S$_2$CN(*i*-Pr)$_2$)]		6660		111
[Co(S$_2$C-(morph))$_2$(S$_2$CN(c-Hex)$_2$)]		6660		111
[Co(S$_2$CN(Bu)(Ph))$_3$]		6660	1830	111
[Co(S$_2$CN)(Hex)$_2$(S$_2$CN(*i*-Pr)$_2$)]		6660		111
[Co$_2$(S$_2$CN(Et)$_2$)$_5$]$^+$ (I)		6660		112
[Co(S$_2$CN(Me)$_2$)$_2$(^{15}NO)] /CDCl$_3$		6668	750	121
[Co(S$_2$CN(Oct)$_2$)$_2$(S$_2$CN(*i*-Pr)$_2$)]		6670		111
[Co(S$_2$CN(Et)$_2$)$_2$(S$_2$CN(*i*-Pr)$_2$)]		6670		111
[Co(S$_2$CN(Et)(3-C$_6$H$_4$OH))$_3$]		6670	2800	111
[Co(Se$_2$CN(*i*-Bu)$_2$)$_3$]		6670		115
[Co(NH$_3$)$_5$CN]$^{2+}$	(21.252 MHz)	6675	2370	93
[Co(S$_2$C-(2-Mepip))$_3$]		6680	1370	111
[Co(S$_2$CN(Et)(Ph))$_3$]		6680	1250	111
[Co(S$_2$CN(Me)$_2$)$_2$(S$_2$CN(c-Hex)$_2$)]		6680		111
[Co$_2$(S$_2$C-(morph))$_5$]$^+$ (I)		6680		112

TABLE 2b (*continued*)

Complex	σ(I)	Width (Hz)	Lit. No.
$[Co(S_2C\text{-}(2\text{-}Mepip))_3]$	6680		112
$[Co(NH_3)_5CN)]^{2+}$	6681		113
$[Co(amben)(^{15}NO)]$ /CD_2Cl_2 (II) (weak)	6687	550	121
$[Co(S_2CN(Me)_2)_2(S_2CN(i\text{-}Pr)_2)]$	6690		111
$[Co(S_2CN(Et)(m\text{-}tol))_3]$	6690	1700	111
$[Co(NH_3)_5CN]^{2+}$	6700	1830	11
$[Co(S_2CN(Me)(i\text{-}Bu))_3]$ /CH_2Cl_2	6700	820	111
$[Co(S_2CN(Me)(i\text{-}Pr))_3]$ /CH_2Cl_2	6700	400	111
$[Co(S_2CN(Me)_2)(S_2CN(i\text{-}Bu)_2)_2]$	6700		111
$[Co(S_2CN(Me)(i\text{-}Pr))_3]$	6700		115
$[Co(S_2CN(Me)_2)_3]$	6704		25
$[Co(S_2CN(Et)(3\text{-}pic))_3]$	6710	1250	111
$[Co(S_2CN(Me)_2)_5]^+$ (I)	6710		112
$[Co(S_2CN(Et)(Bz))_3]$	6725	1770	111
$[Co(S_2CN(Pr)_2)_3]$ /CH_2Cl_2	6740	1200	111
$[Co(S_2CN(Pr)_2)_3]$	6740		112
$[Co(S_2CN(Hex)_2)_3]$ /CH_2Cl_2	6750	2120	111
$[Co(S_2CN(Et)(C_2H_4OH))_3]$	6750	850	111
$[Co(S_2C\text{-}(3\text{-}Mepip))_3]$	6750	1250	111
$[Co(Se_2CN(Me)_2)_3]$	6759		25
$[Co(Se_2CN(CH_2)_5)_3]$	6760	1030	111
$[Co(Se_2CN(Me)(i\text{-}Pr))_3]$	6760		115
$[Co(S_2CN(Oct)_2)_3]$ /CH_2Cl_2	6760	2740	111
$[Co(S_2C\text{-}(4\text{-}Mepip))_3]$	6760		112
$[Co(S_2CN(Me)(Bz))_3]$	6760	1430	111
$[Co(S_2C\text{-}(pip))_3]$	6760		112
$[Co(S_2CN(Bu)_2)_3]$ /CH_2Cl_2	6760	1700	111
$[Co(S_2CN(Am)_2)_3]$ /CH_2Cl_2	6760	1940	111
$[Co(S_2C\text{-}(pip))_3]$	6760		115
$[Co(S_2C\text{-}(4\text{-}Mepip))_3]$	6760	1800	111
$[Co(S_2CN(Me)_2)_2(S_2CN(i\text{-}Bu)_2)]$	6770		111
$[Co(S_2CN(Et)(Bu))_3]$/CH_2Cl_2	6780	1430	111
$[Co(S_2CN(Me)(Oct))_3]$ /CH_2Cl_2	6790	1500	111
$[Co(S_2CN(Et)_2)_3]$	6790		115
$[Co(S_2CN(Et)_2)_3]$ /CH_2Cl_2	6790	850	111
$[Co(S_2CN(Et)_2)_3]$	6790		112
$[Co(S_2CN(Et)(t\text{-}Bu))_3]$ /CH_2Cl_2	6800	1500	111
$[Co(salen)(Me)(NH_2Bz)]$	6800		45
$[Co(S_2C\text{-}(morph))_3]$	6800		112
$[Co(S_2CN(Me)(Bu))_3]$ /CH_2Cl_2	6800	1540	111
$[Co(S_2C\text{-}(morph))_3]$	6800		115
$[Co(NH_3)_5CN]^{2+}$	6800		26
$[Co(S_2C\text{-}(morph))_3]$	6800	1150	111
$[Co(Se_2C\text{-}(pip))_3]$	6820		115
$[Co(salen)(Me)(OH_2)]$ /MeOH	6820		45
$[Co(S_2CN(Me)_2)_3]$	6830		112
$[Co(S_2CN(Me)_2)_3]$	6830		115
$[Co(S_2C\text{-}(pyrr))(S_2CN(Et)(Ph))_2]$	6830		111
$[Co(S_2CN(Me)_2)_3]$ /CH_2Cl_2	6830	570	111
$[Co(dien)_2]^{3+}$, bae, cfd- (***) (21.252 MHZ)	6836	425	93
$[Co(dien)_2]^{3+}$, dab, cfe- (***) (21.252 MHZ)	6836	423	95

TABLE 2b (*continued*)

Complex		σ(1)	Width (Hz)	Lit. No.
$[Co(Se_2CN(Et)_2)_3]$		6840		115
$[Co(S_2C\text{-}(pyrr))(S_2CN(t\text{-}Bu)_2)_2]$		6840		111
$[Co(dien)_2]^{3+}$, dab, cfe-(??) (***)	(94.457 MHz)	6846	435	95
$[Co(Se_2C\text{-}(morph))_3]$		6850		115
$[Co(dien)_2]^{3+}$, dab, cfe-(??) (***)	(59.035 MHz)	6850	428	95
$[Co(NH_3)_2(NO_2)_4]^-$		6860	1000	22
$[Co(NH_3)_4(NO_2)_2]^+$, *cis-*		6880		8
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-*		6880		82
$[Co(NH_3)_2(NO_2)_4]^-$, *trans-*		6880	940	11
$[Co(Se_2CN(Me)_2)_3]$		6890		115
$[Co(acacen)(Me)(NH_2Bz)]$		6900		45
$[Co(S_2CN(Me)_2)_2(^{15}NO)]$ /DMSO-d_6		6906	2150	121
$[Co(S_2C\text{-}(pyrr))(S_2C\text{-}(pip))_2]$		6910		111
$[Co(S_2C\text{-}(pyrr))_2(S_2CN(i\text{-}Pr)_2)]$		6920		111
$[Co(NH_3)_3(NO_2)_3]$, *mer-*		6940		8
$[Co(S_2C\text{-}(pyrr))(S_2CN(Me)_2)_2]$		6950		111
$[Co(NH3)_2(NO_2)_4]^{2-}$, *trans-*		6950		7
$[Co(NH_3)_4(CN)(OH_2)]^{2+}$		6950		32
$[Co(acacen)(Me)(NC_5H_5)]$		6960		45
$[Co(S_2C\text{-}(pyrr))_2(S_3CN(c\text{-}Hex)_2)]$		6960		111
$[Co(dien)_2]^{3+}$, bae, cfd-, (***)	(21.252 MHz)	6968	395	95
$[Co(dien)_2]^{3+}$, cae, bfd-, (***)	(21.252 MHz)	6968	395	93
$[Co(NH_3)_3(NO_2)_3]$, *mer-*		6970	480	11
$[Co(en)_3]^{n+}$ deprotonated		6980		44
$[Co(dien)_2]^{3+}$, bae, cfd-, (***)	(94.457 MHz)	6981	427	95
$[Co(NH_3)_3(NO_2)_3]$, *mer-* /H_2O	(21.252 MHz)	6981	782	96
$[Co(NH_3)_3(NO_2)_3]$, *mer-* /H_2O	(59.035 MHz)	6982	956	96
$[Co(NH_3)_3(NO_2)_3]$, *mer-* /H_2O	(94.457 MHz)	6983	970	96
$[Co(dien)_2]^{3+}$, bae, cfd-, (***)	(59.035 MHz)	6985	420	95
$[Co(dien)(NH_3)_3]^{3+}$, *fac-*		6990		65
$[Co(en)_3]^{3+}$		6990		43
$[Co(NH_3)_3(NO_2)_3]$, *mer-* /MeOH	(21.252 MHz)	6992	595	96
$[Co(NH_3)_3(NO_2)_3]$, *mer-* /MeOH	(94.457 MHz)	6998	1068	96
$[Co(NH_3)_3(NO_2)_3]$, *mer-* /DMSO	(59.035 MHz)	7000	2908	96
$[Co(NH_3)_3(NO_2)_3]$, *mer-* /DMSO	(94.457 MHz)	7000	3336	96
$[Co(NH_3)_3(NO_2)_3]$, *mer-* /MeOH	(59.035 MHz)	7005	832	96
$[Co(NH_3)_3(NO_2)_3]$, *mer-* /DMSO	(21.252 MHz)	7007	2231	96
$[Co(en)_3]^{3+}$		7010		43
$[Co(S_2C\text{-}(pyrr))_2(S_2CN(t\text{-}Bu)_2)]$		7010		111
$[Co(en)_3]^{3+}$		7010		8
$[Co(NH_3)_3(NO_2)_3]$, *mer-* /Me_2CO	(21.252 MHz)	7012	363	96
$[Co(S_2C\text{-}(pyrr))_2(S_2CNEtPh)]$		7020		111
$[Co(NH_3)_3(NO_2)_3]$, *mer-* /Me_2CO	(94.457 MHz)	7023	450	96
$[Co(NH_3)_3(NO_2)_3]$, *mer-* /MeCN	(21.252 MHz)	7026	131	96
$[Co(NH_3)_3(NO_2)_3]$, *mer-* /Me_2CO	(59.035 MHz)	7029	376	96
$[Co_2(S_2C\text{-}(pyrr))_5]^+$ (I)		7030		112
$[Co(dien)_2]^{3+}$, dab, cfe- (*mer*)	(21.252 MHz)	7031	3021	95
$[Co(dien)_2]^{3+}$, dab, cfe- (*mer*)	(59.035 MHz)	7032	3384	95
$[Co(dien)_2]^{3+}$, dab, cfe- (*mer*)	(94.457 MHz)	7032	3468	95
$[Co(NH_3)_3(NO_2)_3]$, *mer*, /MeCN	(94.457 MHz)	7033	314	96
$[Co(NH_3)_3(NO_2)_3]$, *mer*, /MeCN	(59.035 MHz)	7038	182	96

TABLE 2b (*continued*)

Complex		σ(1)	Width (Hz)	Lit. No.
$[Co(S_2C\text{-}(pyrr))_2(S_2C(pip))]$		7060		111
$[Co(S_2C\text{-}(pyrr))_2(S_2CN(Me)_2)]$		7070		111
$[Co(S_2CN(CH_2)_4)_3]$		7074		25
$[Co(phen)_3]^{3+}$		7080	500	22
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-*		7080	500	22
$[Co(NH_3)_4(NO_2)_2]^+$, *cis-*		7080	800	22
$[Co(en)_2Cl_2]^+$, *trans-* (*)		7109		7
$[Co(en)_3]^{3+}$		7120		29
$[Co(en)_3]^{3+}$		7124		86
$[Co(en)_2(dicyandiamide)Cl]^+$		7130		69
$[Co(en)_2(CO_3)]^+$ (*)		7131		7
$[Co(en)_3]^{3+}$		7144		68
$[Co(en)_3]^{3+}$		7144		25
$[Co(en)_3]^{3+}$	(94.457 MHz)	7145	117	95
$[Co(en)_3]^{3+}$	(21.252 MHz)	7146	90	95
$[Co(en)_3]^{3+}$	(94.457 MHz)	7146	100	93
$[Co(en)_3]^{3+}$	(21.252 MHz)	7146	97	93
$[Co(en)_3]^{3+}$	(21.252 MHz)	7146	90	93
$[Co(en)_3]^{3+}$		7147		113
$[Co(en)_3]^{3+}$	(59.035 MHz)	7148	98	95
$[Co(acacen)(Me)(OH_2)]$		7140		45
$[Co(acacen)(Me)(OH_2)]$		7150		45
$[Co(NH_3)_4(NO_2)]^+$, *trans-*		7150		8
$[Co(NH_3)_4(NO_2)_2]^+$, *cis-*		7150	– –	82
$[Co(sacaen)(^{15}NO)]$ /DMSO-d_6		7164	6400	121
$[Co(en)_3]^{3+}$		7177		7
$[Co(NH_3)_3(NO_2)_2Cl]$		7190	– –	82
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-*		7199		7
$[Co(S_2C\text{-}(pyrr))_3]$		7200		115
$[Co(NH_3)_3(NO_2)_3]$, *mer-*		7200	500	22
$[Co(S_2C\text{-}(pyrr))_3]$		7200		112
$[Co(S_2C\text{-}(pyrr))_3]$		7200	1150	111
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-* /H_2O	(59.035 MHz)	7206	356	96
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-* /H_2O	(21.252 MHz)	7207	355	96
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-* /H_2O	(94.457 MHz)	7208	356	96
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-* /CF_3COOH	(94.457 MHz)	7215	2588	96
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-*		7220	270	11
$[Co(pn)_3]^{3+}$ (isomer mixture)		7220		7
$[Co(S_2CNH_2)_3]$		7223		86
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-* /MeOH	(21.252 MHz)	7224	439	96
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-* /DMSO	(21.252 MHz)	7225	888	96
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-* /MeCN	(21.252 MHz)	7228	253	96
$[Co(S_2CNH_2)_3]$		7231		25
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-* /MeCN	(59.035 MHz)	7233	260	96
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-* /DMSO	(59.035 MHz)	7234	1085	96
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-* /DMSO	(94.457 MHz)	7235	1085	96
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-* /MeOH	(94.457 MHz)	7236	487	96
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-* /MeCN	(94.457 MHz)	7238	280	96
$[Co(NH_3)_4(NO_2)_2]^+$, *trans-* /MeOH	(59.035 MHz)	7241	487	96
$[Co(NH_3)_4(NO_2)_2]^+$, *cis-* /H_2O	(59.035 MHz)	7272	356	96

TABLE 2b (*continued*)

Complex	σ(1)	Width (Hz)	Lit. No.
$[Co(NH_3)_4(NO_2)_2]^+$, *cis*- /DMSO (21.252 MHz)	7274	1181	96
$[Co(NH_3)_4(NO_2)_2]^+$, *cis*- /H_2O (94.457 MHz)	7276	440	96
$[Co(NH_3)_4(NO_2)_2]^+$, *cis*- /H_2O (21.252 MHz)	7277	331	96
$[Co(NH_3)_4(NO_2)_2]^+$, *cis*- /CH_3COOH (94.457 MHz)	7279	1595	96
$[Co(NH_3)_4(NO_2)_2]^+$, *cis*-	7280	270	11
$[Co(NH_3)_4(NO_2)_2]^+$, *cis*- /DMSO (59.035 MHz)	7288	1648	96
$[Co(NH_3)_4(NO_2)_2]^+$, *cis*- /DMSO (94.457 MHz)	7290	2310	96
$[Co(NH_3)_4(NO_2)_2]^+$, *cis*-	7290		7
$[Co(en)_2(NH_3)_2]^{3+}$, *cis*-	7300	200	22
$[Co(NH_3)_4(NO_2)_2]^+$, *cis*- /MeOH (21.252 MHz)	7300	326	96
$[Co(en)_3]^{3+}$	7300		5
$[Co(NH_3)_4(NO_2)_2]^+$, *cis*- /MeCN (21.252 MHz)	7301	180	96
$[Co(NH_3)_4(NO_2)_2]^+$, *cis*- /MeCN (59.035 MHz)	7305	230	96
$[Co(NH_3)_4(NO_2)_2]^+$, *cis*- /MeCN(94.457 MHz)	7305	320	96
$[Co(Se_2C\text{-}(pyrr))_3]$	7310		115
$[Co(NH_3)_4(NO_2)_2]^+$, *cis*- /MeOH (94.457 MHz)	7311	700	96
$[Co(NH_3)_4(NO_2)_2]^+$, *cis*- /MeOH (59.035 MHz)	7316	404	96
$[Co(NH_3)_4(NO_2)_2]^+$, *trans*- /MeCN (94.457 MHz)	7328(??)	280	96
$[Co(NO_2)_6]^{3-}$ (**)	7350		82
$[Co(NO_2)_6]^{3-}$ (**)	7350		8
$[Co(en)_2(^{15}NO)]$, *trans*-(I)/Me_2CO	7357	2100	121
$[Co(en)_3]^{3+}$	7380	120	22
$[Co(NH_3)(NO_2)_3(CO_3)]^{2-}$	7400		32
$[Co(NO_2)_6]^{3-}$ (**)	7400		5
$[[Co(tetraen)]_2(O_2)]^{4+}$, (fcdaa',f'bcde')bc'-(***) (21.252 MHz)	7408	2354	93
$[[Co(tetraen)]_2(O_2)]^{4+}$ (b)-I (21.252 MHz)	7408	2354	94
$[[Co(tetraen)]_2(O_2)]^{4+}$, (fcdaa',f'bcde')bc'- (***) (59.035 MHz)	7417	8500	93
$[[Co(tetraen)]_2(O_2)]^{4+}$, (b)-I (59.035 MHz)	7417		94
$[Co(CN)_5NO_2]^{3-}$ (*)	7420		32
$[Co(tame)_2]^{3+}$	7424		113
$[Co(NH_3)_5NO_2]^{2+}$	7440	100	22
$[Co(NO_2)_6]^{3-}$ (**)	7440	300	22
$[Co(NO_2)_6]^{3-}$ (**)	7444		25
$[[Co(tetraen)]_2(O_2)]^{4+}$ (a)-I (21.252 MHz)	7447	777	94
$[[Co(tetraen)]_2(O_2)]^{4+}$, edacf,b- (***) (21.252 MHz)	7447	777	93
$[Co(benacen)(^{15}NO)]$ /$CDCl_3$	7449	5800	121
$[[Co(tetraen)]_2(O_2)]^{4+}$, edacf,b- (***) (94.457 MHz)	7455	958	93
$[[Co(tetraen)]_2(O_2)]^{4+}$, edacf,b- (***) (59.035 MHz)	7456	967	93
$[Co(NO_2)_6]^{3-}$ (***)	7458		68
$[Co(NH_3)_5NO_2]^{2+}$	7460		8
$[[Co(tetraen)]_2(O_2)]^{4+}$, (a)-I (59.035 MHz)	7479	967	94
$[[Co(tetraen)]_2(O_2)]^{4+}$, aedcf,b- (***) (94.457 MHz)	7483	667	93
$[[Co(tetraen)]_2(O_2)]^{4+}$, aedcf,b- (***) (59.035 MHz)	7483	553	93
$[[Co(tetraen)]_2(O_2)]^{4+}$, aedcf,b- (***) (21.252 MHz)	7484	364	93
$[[Co(tetraen)]_2(O_2)]^{4+}$, (a)-II (21.252 MHz)	7484	364	94
$[Co(NH_3)_5NO_2]^{2+}$	7490		15
$[Co(NO_2)_6]^{3-}$ (**)	7490		7
$[[Co(tetraen)]_2(O_2)]^{4+}$, (cfed'e',f'b'a'ad),bc'- (***) (94.457 MHz)	7494	801	93

TABLE 2b (*continued*)

Complex	$\sigma(1)$	Width (Hz)	Lit. No.
$[Co(NH_3)_5ONO]^{2+}$ (*)	7500		15
$[Co(dien)(NH_3)_3]^{3+}$, *mer-*	7500	– –	65
$[[Co(tetraen)]_2(O_2)]^{4+}$ (a)-III (21.252 MHz)	7504	485	94
$[[Co(tetraen)]_2(O_2)]^{4+}$ (a)-II (59.035 MHz)	7508	753	94
$[[Co(en)]_2(NH_3)_2]^{3+}$, *trans-*	7510	400	22
$[[Co(tetraen)]_2(O_2)]^{4+}$ (dfcaa',edeb'f'),bc'- (***) (59.035 MHz)	7515	1721	93
$[[Co(tetraen)]_2(O_2)]^{4+}$ (dfcaa',edeb'f'),bc'- (***) (21.252 MHz)	7516	970	93
$[[Co(tetraen)]_2(O_2)]^{4+}$ (dfcaa',edeb'f'),bc'- (***) (94.457 MHz)	7518	1621	93
$[[Co(tetraen)]_2(O_2)]^{4+}$ (a)-III (59.035 MHz)	7520	1721	94
$[Co(NH_3)_5NO_2]^{2+}$	7520		82
$[[Co(tetraen)]_2(O_2)]^{4+}$ (a)-IV (21.252 MHz)	7527	485	94
$[[Co(tetraen)]_2(O_2)]^{4+}$ (a)-IV (59.035 MHz)	7539	1721	94
$[[Co(dien)(en)]_2(O_2)]^{4+}$, abf,de,c- (***) (59.035 MHz)	7552	846	94
$[[Co(dien)(en)]_2(O_2)]^{4+}$, edf,ac,b-(***) (59.035 MHz)	7552	846	93
$[[Co(tetraen)]_2(O_2)]^{4+}$, (dfcaa',edeb'f'),bc'- (***) (94.457 MHz)	7552	3858	93
$[[Co(dien)(en)]_2(O_2)]^{4+}$ edf,ac,b- (***) (94.457 MHz)	7554	1282	93
$[[Co(dien)(en)]_2(O_2)]^{4+}$, abf,de,c- (***) (94.457 MHz)	7554	1282	94
$[[Co(dien)(en)]_2(O_2)]^{4+}$, abf,de,c- (***) (21.252 MHz)	7555	760	94
$[[Co(dien)(en)]_2(O_2)]^{4+}$, edf,ac,b- (***) (21.252 MHz)	7555	760	94
$[[Co(tetraen)]_2(O_2)]^{4+}$, deacf, b- (***) (59.035 MHz)	7560		93
$[[Co(dien)(en)]_2(O_2)]^{4+}$, def,ac,b- (***) (94.457 MHz)	7568	1661	93
$[[Co(tetraen)]_2(O_2)]^{4+}$, (b)-II (21.252 MHz)	7569	1311	94
$[[Co(dien)(en)]_2(O_2)]^{4+}$, def,ac,b- (***) (59.035 MHz)	7569	924	93
$[[Co(dien)(en)]_2(O_2)]^{4+}$, ebf,ad,c- (***) (59.035 MHz)	7569	924	94
$[[Co(tetraen)]_2(O_2)]^{4+}$, deacf,b- (***) (21.252 MHz)	7569	1311	93
$[[Co(dien)(en)]_2(O_2)]^{4+}$, ebf,ad,c- (***) (21.252 MHz)	7572	850	94
$[[Co(dien)(en)]_2(O_2)]^{4+}$, def,ac,b- (***) (21.252 MHz)	7572	850	93
$[[Co(tetraen)]_2(O_2)]^{4+}$, deacf, b- (***) (94.457 MHz)	7576	2386	93
$[Co(NH_3)_5NO_2]^{2+}$	7576	440	94
$[Co(dbzm\text{-}S)_3]$, *fac*-/C_6H_6	7580		105
$[[Co(tetraen)]_2(O_2)]^{4+}$ (b)-II (59.035 MHz)	7584	4087	94
$[[Co(tetraen)]_2(O_2)]^{4+}$, (cfed'e',f'b'a'ad),bc'- (***) (94.457 MHz)	7594	3932	93

TABLE 2b (*continued*)

Complex	$\sigma(1)$	Width (Hz)	Lit. No.
$[Co(C_2O_4)_3]^{3-}$ (*)	7610		27
$[Co(en)_2(^{15}NO)]$, *trans*-(II) /Me_2CO	7612	2600	121
$[[Co(tetraen)]_2(O_2)]^{4+}$, (acff',a'e'd'ed),bc'- (***) (21.252 MHz)	7614	2985	93
$[[Co(tetraen)]_2(O_2)]^{4+}$ (b)-III (21.252 MHz)	7614	2985	94
$[Co(NH_3)_5NO_2]^{2+}$	7620	170	11
$[Co(NO_2)_6]^{3-}$ (**)	7630	50	10
$[[Co(tetraen)]_2(O_2)]^{4+}$ (acff',a'e'd'ed),bc'- (***) (59.035 MHz)	7632	7632	93
$[[Co(tetraen)]_2(O_2)]^{4+}$ (acff',a'e'd'ed),bc'- (***) (94.457 MHz)	7640	6386	93
$[Co(NH_3)_5NO_2]^{2+}$	7642		113
$[[Co(dien)(en)]_2(O_2)]^{4+}$, aef,cd,b- (***) (94.457 MHz)	7650	3560	93
$[[Co(dien)(en)]_2(O_2)]^{4+}$, bcf,ad,c- (***) (94.457 MHz)	7650	3560	94
$[[Co(dien)(en)]_2(O_2)]^{4+}$, bcf,ad,c- (***) (21.252 MHz)	7652	1453	94
$[[Co(dien)(en)]_2(O_2)]^{4+}$, aef,cd,b- (***) (21.252 MHz)	7652	1453	93
$[[Co(dien)(en)]_2(O_2)]^{4+}$, bcf,ad,c- (***) (59.035 MHz)	7654	2231	94
$[[Co(dien)(en)]_2(O_2)]^{4+}$ aef,cd,b- (***) (59.035 MHz)	7654	2231	93
$[[Co(trien)NH_3]_2(O_2)]^{4+}$, e,c(adf),b- (***) (21.252 MHz)	7655	1913	93
$[[Co(NH_3)(trien)]_2(O_2)]^{4+}$, b,e(adf),c-(pH 10.5) (***) (21.252 MHz)	7655	1913	94
$[Co(salen)(^{15}NO)]/CDCl_3$	7658	11700	121
$[[Co(NH_3)(trien)]_2(O_2)]^{4+}$, b,e(adf),c-(pH 4.75) (***) (21.252 MHz)	7672	1766	94
$[Co(trien)(NH_3]_2(O_2)]^{4+}$, e,c(adf),b- (***) (21.252 MHz)	7672	1766	93
$[Co(tetraen)]_2(O_2)]^{4+}$, (b)-III (59.035 MHz)	7720	– –	94
$[Co(en)(dien)Cl]^{2+}$, df,abe,c- (***) (21.252 MHz)	7758	2787	93
$[Co(en)(NH_3)_4]^{3+}$, *cis*-	7843	325	93
$[Co(NH_3)_5NO]^{2+}$ (94.457 MHz)	7865	188	95
$[Co(NH_3)_5NO]^{2+}$ (21.252 MHz)	7867	141	95
$[Co(NH_3)_5NO]^{2+}$ (59.035 MHz)	7869	162	95
$[Co(TPP)(^{15}NO)]/CD_2Cl_2$	7909	4250	121
$[Co(en)(dien)Cl]^{2+}$, de,abf,c- (***) (21.252 MHz)	7964	3194	93
$[Co(acacen)(^{15}NO)]$ /DMSO-d_6	8001	1700	121
$[Co(en)_2Cl(NH_2Me)]^{2+}$	8010		88
$[Co(en)_2(NC_5H_5)Cl]^{+}$	8030		69
$[Co(NO_2)_6]^{3-}$ (**)	8060		7
$[Co(salen)(NH_3)_2]^{+}$	8060		45
$[Co(NH_3)_6]^{3+}$	8080		8
$[Co(NH_3)_6]^{3+}$	8100		32
$[Co(NH_3)_6]^{3+}$	8100		14

TABLE 2b (*continued*)

Complex		$\sigma(1)$	Width (Hz)	Lit. No.
$[Co(NH_3)_6]^{3+}$		8100		27
$[Co(NH_3)_6]^{3+}$		8100		32
$[Co(NH_3)_6]^{3+}$		8100		82
$[Co(NH_3)_6]^{3+}$		8100	220	22
$[Co(NO_2)_6]^{3-}$ (**)		8100		5
$[Co(salen)(^{15}NO)]$/DMSO-d_6		8100		121
$[Co(NH_3)_6]^{3+}$		8114		86
$[Co(NH_3)_5)(S_2O_3)]^+$		8117		113
$[[Co(en)_2(NCS)]_2(O_2)]^{2+}$, ad,cf,e,b-	(21.252 MHz)	8131	2231	93
$[[Co(en)_2(NCS)]_2(O_2)]^{2+}$, ad,cf,e,b-	(94.457 MHz)	8134	2522	93
$[Co(NO_2)_6]^{3-}$ (**)		8160	400	22
$[Co(en)_2(SCN)_2]^+$, ad,cf,b,e-	(21.252 MHz)	8161	1144	93
$[Co(benacen)(^{15}NO)]$ /CD_2Cl_2		8170	2550	121
$[Co(NH_3)_5(HIm)]^{3+}$		8170	230	116
$[Co(NH_3)_6]^{3+}$ $-\{^{15}N_6\}$		8171		68
$[Co(NH_3)_6]^{3+}$		8174	183	95
$[Co(NH_3)_6]^{3+}$		8175		25
$[Co(NH_3)_6]^{3+}$		8175	172	95
$[Co(NH_3)_6]^{3+}$		8175	172	93
$[Co(NH_3)_6]^{3+}$		8176	183	95
$[Co(NH_3)_5SCN]^{2+}$		8177		113
$[Co(NH_3)_6]^{3+}$		8178		68
$[Co(NH_3)_5(MeIm)]^{3+}$		8178	240	116
$[Co(en)_2$(*m*-tol)$Cl]^+$		8180		69
$[Co(en)_2Cl(NH_2C_6H_4OMe$, *o*-$)]^{2+}$		8180		88
$[Co(NH_3)_4(NO_2)Cl]^{2+}$, *trans*-		8180		82
$[Co(en)_2$(*m*-anisidine)$Cl]^+$		8180		69
$[Co(NH_3)_5NCS]^{2+}$		8200		15
$[Co(NH_3)_6]^{3+}$		8206		113
$[Co(NH_3)_5(HIm)]^{3+}$/MeOH		8208	350	116
$[Co(en)_2$(*p*-anisidine)$Cl]^+$		8210		69
$[Co(en)_2$(*m*-chloroaniline)$Cl]^+$		8210		69
$[Co(NH_3)_5(MeIm)]^{3+}$/MeOH		8215	390	116
$[Co(NH_3)_6]^{3+}$		8218		7
$[Co(en)_2$(*o*-phenetidine)$Cl]^+$		8220		69
$[Co(en)_2Cl(NH_2C_6H_4Me$, *p*-$)]^{2+}$		8230		88
$[Co(NH_3)_5(NC_5H_5)]^{3+}$ /Me_2CO		8245	2200	116
$[Co(en)_2Cl(NH_2C_6H_4OEt$, *p*-$)]^{2+}$		8260		88
$[Co(en)_2Cl(NH_2Ph)]^{2+}$		8260		88
$[Co(NH_3)_5(NC_5H_5)]^{3+}$ /MeOH		8272	1700	116
$[[Co(en)_2(NCS)]_2(O_2)]^{2+}$, ae,cf,d,b-	(94.457 MHz)	8279	4964	93
$[Co(NH_3)_4(OH_2)(NO_2)]^{2+}$, *cis*-		8300	– –	82
$[Co(TPP)(HIm)_2]^+$/MeOH(ClO_4)		8300	500	116
$[Co(en)_2$(*m*-phenetidine)$Cl]^+$		8300		69
$[Co(TPP)(HIm)_2]^+$/MeOH(BF_4)		8300	430	116
$[Co(NH_3)_5(OH_2)]^{3+}$		8300		14
$[Co(NH_3)_6]^{3+}$		8300		5
$[Co(acacen)(NH_3)_2]^+$		8300		45

TABLE 2b (*continued*)

Complex		σ(I)	Width (Hz)	Lit. No.
$[Co(TPP)(HIm)_2]^+$ /MeOH(BPh_4)		8302	700	116
$[Co(NH_3)_5(OH_2)]^{3+}$		8310		15
$[Co(tn)_3]^{3+}$		8312		86
$[Co(en)(NCS)_2SCN]_2(en)]$, ad,bc,f,e-	(94.457 MHz)	8313	871	93
$[Co(NH_3)_5NCS]^{2+}$		8328	196	93
$[Co(pn)_3]^{3+}$ (isomer mixture)		8339		68
$[Co(TPP)(HIm)_2]^+$ /MeCN (ClO_4)		8345	330	116
$[Co(NH_3)_5NCS]^{2+}$		8345		113
$[Co(NH_3)(NO_2)_3(C_2O_4)]^{2-}$		8350		32
$[Co(NH_3)_6]^{3+}$		8350	ca. 50	10
$[Co(en)(NCS)_2SCN]_2(en)]$, cd,af,b,e-	(94.457 MHz)	8350	12064	93
$[Co(NH_3)_2(C_2O_4)(NO_2)_2]^-$		8350		27
$[Co(TPP)(MeIm)_2]^+$ /MeOH(BPh_4)		8354	1000	116
$[Co(TPP)(MeIm)_2]^+$ /MeOH(BF_4)		8355	920	116
$[Co(TPP)(MeIm)_2]^+$ /MeOH(ClO_4)		8355	860	116
$[Co(TPP)(HIm)_2]^+$ /$C_2H_4Cl_2$(ClO_4)		8360	1600	116
$[Co(TPP)(HIm)_2]^+$ /Me_2CO(ClO_4)		8360	330	116
$[[Co(salen)]_2O_2(H_2O)_2]$		8365	13249	93
$[[Co(salen)]_2O_2(DMSO)_2]$		8367	13287	93
$[[Co(salen)]_2O_2(DMSO)_2]$		8367	13287	94
$[Co(TPP)(MeIm)_2]^+$ /MeCN(ClO_4)		8368	500	116
$[[Co(salen)]_2O_2(DMSO)_2]$		8369	12854	93
$[[Co(salen)]_2O_2(DMSO)_2]$		8369	12854	94
$[[Co(salen)]_2O_2(DMF)_2]$		8375	13624	93
$[[Co(salen)]_2O_2(H_2O)_2]$		8381	13158	93
$[[Co(en)_2(SCN)]_2(O_2)]^{2+}$, ae,df,b,c-	(59.035 MHz)	8385	1266	94
$[[Co(en)_2(SCN)]_2(O_2)]^{2+}$, ad,cf,e,b-	(94.457 MHz)	8389	1400	93
$[[Co(TPP)(HIm)_2]^+$ /CH_2Cl_2(ClO_4		8389	1000	116
$[[Co(en)_2(SCN)]_2(O_2)]^{2+}$, ae,df,b,c-	(94.457 MHz)	8391	2500	94
$[Co(TPP)(MeIm)_2]^+$ /$C_2H_4Cl_2$(ClO_4)		8392	1600	116
$[Co(TPP)(HIm)_2]^+$ /THF(ClO_4)		8392	660	116
$[[Co(en)_2(SCN)]_2(O_2)]^{2+}$, ad,cf,e,b-	(21.252 MHz)	8396	1230	93
$[Co(TPP)(MeIm)_2]^+$ /THF(ClO_4)		8401	1000	116
$[Co(TPP)(MeIm)_2]^+$ /Me_2CO(ClO_4)		8409	500	116
$[Co(TPP)(MeIm)_2]^+$ /CH_2Cl_2(ClO_4)		8443	1000	116
$[Co(NH_3]_5NH_2OSO_2]^{2+}$		8444		113
$[Co(3\text{-}MeOsalox)_2(^{15}NO)]$ /DMSO-d_6		8446	16800	121
$[Co(ketox)(^{15}NO)]$ /$CDCl_3$		8478	240	121
$[[Co(en)_2(SCN)]_2(O_2)]^{2+}$, ab,df,e,c-	(95.457 MHz)	8499	6163	94
$[[Co(en)_2(SCN)]_2(O_2)]^{2+}$, ae,cf,d,b-	(94.457 MHz)	8501	13646	93
$[[Co(en)_2(SCN)]_2(O_2)]^{2+}$, ab,df,e,c-	(59.035 MHz)	8502	4700	94
$[[Co(NH_3)_3](OH)(NO_2)_2]^{3+}$, $\{CoN_4O_2\}$		8520	4150	56

TABLE 2b (*continued*)

mplex		σ(I)	Width (Hz)	Lit. No.
$(salox)(^{15}NO)]$ /$CDCl_3$		8586	3000	121
$(en)(NCS)_2](en)(O_2)]$, ac,df,e,b-	(94.457 MHz)	8591	6951	93
$(en)(NCS)_2](en)(O_2)]$, ac,df,c,b-	(21.252 MHz)	8597	1742	93
$(NH_3)_5SCN]^{2+}$	(21.252 MHz)	8600	784	93
$(en)(NCS)(SCN)]_2(en)(O_2)]$, ad,c,f,e,b-	(94.457 MHz)	8664	7023	93
$(en)_2Cl(NH_2C_6H_4OMe$, p-$)]^{2+}$		8670		88
$(NH_2(CH_2)_4NH_2)_3]^{3+}$		8670		97
$(NH_3)_5(N_3)]^{2+}$	(21.252 MHz)	8671	172	94
$(NH_3)_5(N_3)]^{2+}$		8681		113
$(NH_3)_5ONO]^{2+}$		8700		82
$(NH_3)_5F]^{2+}$		8710		15
$(NH_3)_5Br]^{2+}$		8710		15
$(en)_2$(*o*-chloroaniline)$Cl]^+$		8710		69
$(NH_3)_5OSO_3H]^{2+}$		8720		15
$(en)_2(C_2O_4)]^+$		8731		113
$(NH_3)_5OSO_3]^+$		8750		15
$(NH_3)_5Cl]^{2+}$		8750		15
$(OEP)(HIm)_2]^+$ /$MeOH(BF_4)$		8753	130	116
$(en)_2Cl_2]^+$, *trans-* /MeCN	(21.252 MHz)	8754	3672	96
$(NH_3)_5]_2(O_2)]^{4+}$ /6M NH_4OH	(21.252 MHz)	8759	1172	93
$(NH_3)_5]_2(O_2)]^{4+}$ /6M NH_4OH	(21.252 MHz)	8759	1172	94
$(NH_3)_5I]^{2+}$	(21.252 MHz)	8760		94
$(NH_3)_3](OH)_2(NO_2)]^{3+}$, $[CoN_4O_2]$		8760	540	56
$(NH_3)_5SCN]^{2+}$		8760		15
$(NH_3)_5I]^{2+}$		8760	2100	29
$(en)_2(N_3)_2]^+$, *cis-*	(21.252 MHz)	8763	986	93
$(en)_2Br_2]^+$, *cis-*	(21.252 MHz)	8764	5420	93
$(en)_2Cl_2]^+$, *trans-* /MeCN	(94.457 MHz)	8788	5100	96
$(en)_2Cl_2]^+$, *trans-* /MeCN	(59.035 MHz)	8797	4000	96
$(OEP)(MeIm)_2]^+$ /$MeOH(BF_4)$		8810	230	116
$(NH_3)_5Br]^{2+}$		8820	1750	29
$(NH_3)_5Br]^{2+}$		8820		94
$(NH_3)_5(N_3)]^{2+}$		8821	324	93
$(en)_2Cl_2]^+$, *trans-* /MeOH	(94.457 MHz)	8821	12920	96
$(en)_2Cl_2]^+$, *trans-* /MeOH	(94.457 MHz)	8821	12920	95
$(NH_3)_5Br]^{2+}$		8823	1317	93
$(en)_2Cl_2]^+$, *trans-* /MeOH	(21.252 MHz)	8837	9375	95
$(NH_3)_5Cl]^{2+}$		8840	950	11
$(en)_2Cl_2]^+$, *trans-* /DMSO	(94.457 MHz)	8841	17660	96
$(NH_3)_5I]^{2+}$		8849		113
$(NH_3)_5Cl]^{2+}$		8850	1750	29
$(en)_2Cl_2]^+$, *trans-* /MeOH	(59.035 MHz)	8855	10209	96
$(en)_2Cl_2]^+$, *trans-* /MeOH	(59.035 MHz)	8855	10209	95
$(en)_2(mal)]^+$		8870		113
$(en)_2Cl_2]^+$, *trans-* /MeOH	(21.252 MHz)	8873	9375	96
$(S_2P(OEt)_2]_3$		8880		17
$(NH_3)_5Cl]^{2+}$	(21.252 MHz)	8887	1460	95
$(NH_3)_5Cl]^{2+}$	(21.252 MHz)	8887	1146	94

TABLE 2b (*continued*)

Complex		σ(I)	Width (Hz)	Lit. No.
$[Co(NH_3)_5Cl]^{2+}$	(21.252 MHz)	8887	1460	93
$[Co(en)_2CO_3]^+$	(21.252 MHz)	8888	2968	93
$[Co(NH_3)_5Cl]^{2+}$		8889		113
$[Co(NH_3)_5Cl]^{2+}$	(59.035 MHz)	8890	1882	95
$[Co(NH_3)_5Cl]^{2+}$	(94.457 MHz)	8890	1851	95
$[Co(NH_3)_5Cl]^{2+}$	(59.035 MHz)	8890	1914	94
$[Co(NH_3)_5Cl]^{2+}$	(94.457 MHz)	8890	2887	94
$[Co(en_2Cl_2]^+$, *trans*-/DMSO	(59.035 MHz)	8897	14180	96
$[Co(NH_3)_5OCOMe]^{2+}$		8910		15
$[Co(NH_3)_5Br]^{2+}$		8919		113
$[Co(NH_3)_5ONO_2]^{2+}$		8930		15
$[Co(NH_3)_5I]^{2+}$		8940		15
$[Co(en)_2(C_2O_4)]^+$		8960	3000	22
$[Co(en)_2Cl_2]^+$, *trans*- /H_2O	(94.457 MHz)	8960	16783	96
$[Co(en)_2Cl_2]^+$, *trans*- /H_2O	(94.457 MHz)	8960	16783	95
$[Co(salox)(^{15}NO)]$ /DMSO-d_6		8966	2700	121
$[Co(en)_2Cl_2]^+$, *cis*-	(21.252 MHz)	8966	5126	95
$[Co(en)_2Cl_2]^+$, *cis*-	(59.035 MHz)	8968	8483	95
$[Co(en)_2Cl_2]^+$, *cis*-	(21.252 MHz)	8974	5126	93
$[Co(S_2P(OEt)_2)_3]$		8978		25
$[Co(NH_3)_4(ONO)_2]^+$, *cis*-		8980		82
$[Co(en)_2Br_2]^+$, *trans*-	(21.252 MHz)	8982	7453	93
$[Co(en)_2Cl_2]^+$, *cis*-	(94.457 MHz)	8987	9218	95
$[Co(en)_2Cl_2]^+$, *trans*-		9000		26
$[Co(NH_3)_5OCO_2]^+$		9000		32
$[Co(NH_3)_5OCO_2H]^{2+}$		9000		15
$[Co(NH_3)_5OCO_2]^+$		9000		8
$[Co(S_2P(OEt)_2)_3]$		9048		113
$[Co(NH_3)_5(OH_2)]^{3+}$		9060		29
$[Co(NH_3)_5OCO_2]^+$	(21.252 MHz)	9062	1947	95
$[Co(NH_3)_5OCO_2]^+$	(21.252 MHz)	9062	1947	93
$[Co(NH_3)_5Cl]^{2+}$		9070		8
$[Co(NH_3)_4CO_3]^{2+}$		9070		8
$[Co(en)_2Cl(NH_2Et)]^{2+}$		9080		88
$[Co(NH_3)_5OCO_2]^{2+}$	(94.457 MHz)	9084	5395	95
$[Co(NH_3)_5OCO_2]^{2+}$	(59.035 MHz)	9090	3383	95
$[Co(en)_2(N_3)_2]^+$, *trans*-	(21.252 MHz)	9092	3500	93
$[Co(7\text{-Mesalen})(^{15}NO)]$ /CD_2Cl_2		9100	2250	121
$[Co(NH_3)_5(OH_2)]^{3+}$		9100	2430	11
$[Co(NH_3)_5(N_3)]^{2+}$		9100	300	22
$[[Co(NH_3)_3](OH)_2(C_2O_4Co(NH_3)_5)]^{5+}$	$\{CoN_5O\}$	9100	broad	56
$[[Co(NCS)_4(SCN)]_2(en)]^{4-}$, acdf,b,e-	(21.252 MHz)	9101	180	93
$[[Co(NCS)_4(SCN)]_2(en)]^{4-}$, bcde,a,f-	(21.252 MHz)	9101	180	93
$[Co(NH_3)_5(O_2CMe)]^{2+}$		9107		113
$[Co(NH_3)_5(OH_2)]^{3+}$	(94.457 MHz)	9114	4405	94
$[Co(NH_3)_5(OH)^{2+}$		9117		29
$Co(NH_3)_5(OH)]^{2+}$		9120	1150	11
$[Co(NH_3)_5(OH_2)]^{3+}$	(21.252 MHz)	9122	4005	94
$[Co(en)(SCN)_3NCS]^-$, cd,abe,f-	(21.252 MHz)	9124	302	93

TABLE 2b (*continued*)

Complex		σ(1)	Width (Hz)	Lit. No.
$[Co(NH_3)_5(OH_2)]^{3+}$	(59.035 MHz)	9130	3977	94
$[Co(NH_3)_5(C_2O_4)]^+$		9130		27
$[Co(NH_3)_4CO_3)^+$		9146		7
$[Co(NH_3)_5(OH_2)]^{3+}$		9147		113
$[Co(NH_3)_5(OH_2)]^{3+}$		9147	4196	93
$[Co(en)_2Cl_2]^+$, *trans-* /H_2O	(59.035 MHz)	9163	13400	95
$[Co(en)_2Cl_2]^+$, *trans-* /H_2O	(59.035 MHz)	9163	13400	96
$[Co(NH_3)_4(N_3)_2]^+$, *trans-*		9170	500	22
$[Co(NH_3)_5(OH_2)]^{3+}$		9170	3000	22
$[[Co(NH_3)_4]_2(OH)_2]^{4+}$		9180	170	56
$[Co(en)_2CO_3]^+$		9180	3000	22
$[Co(NH_3)_5OCO_2]^+$		9184	5395	95
$[Co(NCS)_6]^{3-}$		9187	158	93
$[Co(NH_3)_4(C_2O_4)]^+$		9190		27
$[Co(NH_3)_5OH]^{2+}$		9196		113
$[Co(en)_2Cl(NH_2CH(Me)_2)]^{2+}$		9210		88
$[Co(salphen)(^{15}NO)]$ /DMSO-d_6		9300	5700	121
$[Co(en)_2Cl_2]^+$, *trans-* /H_2O	(21.252 MHz)	9333	8597	95
$[Co(en)_2Cl_2]^+$, *trans-*	(21.252 MHz)	9333	8597	93
$[Co(en)_2Cl_2]^+$, *trans-* /H_2O	(21.252 MHz)	9333	8597	96
$[[Co(NH_3)_4]_2(NH_2)(OH)]^{4+}$		9388		56
$[Co(ketox)(^{15}NO)]$ /DMSO-d_6		9390	4000	121
$[Co(NH_3)_4(N_3)_2]^+$, *cis-*		9400	300	22
$[Co(NH_3)_4(N_3)_2]^+$, *cis-*		9448	385	93
$[Co(acac)(dbzm\text{-}S)_2]$,*cis*(S)-Cl-		9450		105
$[Co(NH_3)_5F]^{2+}$		9520		29
$[Co(NH_3)_4(OH_2)Cl]^{2+}$		9600		14
$[Co(NH_3)_4CO_3]^+$		9620		32
$[Co(3\text{-}MeOsalox)_2(^{15}NO)]$ /CD_2Cl_2		9623	2600	121
$[Co(NH_3)_4Cl_2]^+$, *cis-*		9630	3400	93
$[Co(NH_3)_4CO_3]^+$		9680	3000	22
$[Co(NH_3)_5F]^{2+}$		9701		113
$[Co(NH_3)_4(OH_2)(ONO)]^{2+}$, *cis-*		9710		82
$[[Co(NH_3)_3](OH)_2NO_2)]^{3+}$, $\{CoN_3O_3\}$		9729	5476	95
$[Co(NH_3)_4CO_3]^+$		9730	700	11
$[Co(NH_3)_4CO_3]^+$		9732	3291	95
$[Co(NH_3)_4CO_3]^+$, *cis-*		9732	3291	93
$[Co(NH_3)_4CO_3]^+$		9734		7
$[[Co(NH_3)_3](OH)_2(NO_2)]^{3+}$, $\{CoN_3O_3\}$		9735	5173	95
$[Co(NH_3)_4CO_3]^+$		9735		51
$[Co(NH_3)_4CO_3]^+$		9800		26
$[Co(NH_3)_4Cl_2]^+$, *trans-*		9808	5857	93
$[Co(NH_3)_4(OH_2)_2]^{3+}$		9820	3000	22
$[Co(5\text{-}Clsalox)_2(^{15}NO)]$ /DMSO-d_6		9890	9000	121
$[Co(NH_3)_3(N_3)_3]$, *fac-*		9917	250	93
$[Co(dien)Cl_3]$, *mer-*		9968	2080	93
$[Co(NH_3)_4(OH_2)]^{3+}$, *cis*-(?)		9980	2610	11
$[[Co(NH_3)_3](OH)_2(NO_2)]^{3+}$, $\{CoN_3O_3\}$		10040	2510	56
$[[Co(NH_3)_4(OH)_2]_3Co]^{6+}$, ligand $\{CoN_4O_2\}$		10060	6230	56
$[Co(NH_3)_3(C_2O_4)Cl]$		10080		27

TABLE 2b (*continued*)

Complex	σ(1)	Width (Hz)	Lit. No.
$[Co(edta)]^-$	10300	4000	22
$[Co(NH_3)_2(C_2O_4)_2]^-$	10400		27
$[[Co(NH_3)_3]_2(OH)_3]^{3+}$	10410	770	56
$[[Co(NH_3)_3](OH)_2(NO_2)]^{3+}$, $\{CoN_3O_3\}$	10480	5860	56
$[[Co(NH_3)_3](OH)_2(\mu\text{-}C_4H_2O_2Co(NH_3)_5)]^{5+}$	10500	2320	56
$[[Co(NH_3)_3](OH)_2(\mu\text{-fumarato})]^{2+}$	10500	2300	56
$[Co(NH_3)_3(OH_2)_3]^{3+}$, *fac-*	10500	350	22
$[[Co(NH_3)_3]_2(OH)_2O_2C(3\text{-}Py)]^{3+}$	10505	3320	57
$[[Co(NH_3)_2(OH)_2O_2CCF_3]^{3+}$	10510	3960	57
$[[Co(NH_3)_3]_2(OH)_2O_2CCHF_2]^{3+}$	10510	2370	57
$[[Co(NH_3)_3]_2(OH)_2O_2CCH_2Br]^{3+}$	10515	1710	57
$[[Co(NH_3)_3]_2(OH)_2O_2C(3\text{-}C_6H_4NO_2)]^{3+}$	10515	2490	57
$[[Co(NH_3)_3]_2(OH)_2O_2C(4\text{-}C_6H_4NO_2)]^{3+}$	10515	2540	57
$[[Co(NH_3)_3]_2(OH)_2O_2C(4\text{-}Py)]^{3+}$	10515	3200	57
$[[Co(NH_3)_3]_2(OH)_2O_2C(2\text{-}Py)]^{3+}$	10515	3570	57
$[[Co(NH_3)_3]_2(OH)_2O_2CCH_2I]^{3+}$	10515	1470	57
$[[[Co(NH_3)_3]_2(OH)_2(O_2C)]_2(CH{=}CH)]^{6+}$	10520	3170	56
$[[(Co(NH_3)_3]_2(OH)_2(C_2O_4Co(NH_3)_5)]^{5+}$	10520	3600	56
$[[Co(NH_3)_3]_2(OH)_2O_2CCHBr_2]^{3+}$	10520	2830	57
$[[Co(NH_3)_3]_2(OH)_2(C_2O_4)]^{2+}$	10520	2490	56
$[[Co(NH_3)_3]_2(OH)_2O_2C(3\text{-}C_6H_4OH)]^{3+}$	10525	1860	57
$[[Co(NH_3)_3]_2(OH)_2O_2CCHCl_2]^{3+}$	10525	2780	57
$[[Co(NH_3)_3]_2(OH)_2O_2CEt]^{3+}$	10525	740	57
$[[Co(NH_3)_3]_2(OH)_2O_2CH]^{3+}$	10525	980	57
$[[Co(NH_3)_3]_2(OH)_2O_2C(4\text{-}C_6H_4OH)]^{3+}$	10525	1660	57
$[[Co(NH_3)_3]_2(OH)_2O_2CMe]^{3+}$	10530	740	57
$[[Co(NH_3)_3]_2(OH)_2O_2CBu]^{3+}$	10530	810	57
$[[Co(NH_3)_3]_2(OH)_2O_2CCH_2Cl]^{3+}$	10530	1640	57
$[[Co(NH_3)_3]_2(OH)_2O_2C(4\text{-}C_6H_4COOMe)]^{3+}$	10535	2830	57
$[[Co(NH_3)_3]_2(OH)_2O_2CCH_2F)]^{3+}$	10535	1560	57
$[[Co(NH_3)_3]_2(OH)_2O_2CCCl_3]^3+$	10535	4220	57
$[[Co(NH_3)_3]_2(OH)_2O_2CCH_2OH]^{3+}$	10540	1320	57
$[[Co(NH_3)_3]_2(OH)_2O_2CCBr_3]^{3+}$	10545	5000	57
$[[Co(en)(C_2O_4)_2]^-$	10572		113
$[Co(NH_3)_3(OH_2)_2Cl]^{2+}$	10600		14
$[Co(en)(mal)_2]^-$	10879		113
$[[Co(NH_3)_3](OH)_2(O_2SO)]^{2+}$, $\{CoN_3O_3\}$	10910	440	56
$[Co(acac)_2(dbzm\text{-}S)]$ /C_6H_6	11350		105
$[Co(NH_3)_2(CO_3)_2]^-$	11500	3000	22
$[Co(NH_3)_2(CO_3)_2]^-$, *cis-*	11626	820	93
$[Co(NH_3)_3(CO_3)Cl]$	11650		32
$[Co(NH_3)_2(CO_3)_2]^-$	11740		32
$[Co(NH_3)_2(OH_2)_3Cl]^{2+}$	11800		14
$[Co(NH_3)_2(CO_3)_2]^-$, *trans-*	11933	4274	93
$[Co(acac)_3]$ /$CHCl_3$	12300		8
$[Co(acac\text{-}NO_2)_3]$	12394		68
$[Co(bzac)_3]$	12400	500	22
$[Co(dbzm)_3]$	12400	500	22
$[Co(tfac)_3]$	12500	160	22
$[Co(acac\text{-}Br)_3]$ /$CHCl_3$	12500	500	22
$[Co(acac)_3]$ /$CHCl_3$	12500	110	22

TABLE 2b (*continued*)

Complex	σ(1)	Width (Hz)	Lit. No.
$[Co(acac)_3]$ /$CHCl_3$	12520		25
$[Co(acac)_3]$ /$CHCl_3$	12529		68
$[Co(dbzm)_3]$ /C_6H_6	12530		105
$[Co(N_3)_6]^{3-}$	12532	207	93
$[Co(Mo_6O_{24}H_6]^{3-}$	12551		113
$[Co(acac)_3]$ /C_6H_6	12630	50	10
$[Co(acac)_3]$ /$CHCl_3$	12650		105
$[Co(acac)_3]$ /C_6H_6	12680		7
$[Co(trop)_3]$	12716		68
$[Co(acac)_3]$ /toluene	12730	50	10
$[Co(acac)_3]$ /Me_2CO	12800	50	10
$[Co(C_2O_4)_3]^{3-}$	12962		86
$[Co(C_2O_4)_3]^{3-}$	12976		25
$[Co(C_2O_4)_3]^{3-}$	12987		113
$[Co(C_2O_4)_3]^{3-}$	13000	250	22
$[Co(C_2O_4)_3]^{3-}$	13000		5
$[Co(C_2O_4)_3]^{3-}$	13040		7
$[Co(CO_3)_3]^{3-}$	13900	250	22
$[Co(CO_3)_3]^{3-}$	13950		32
$[Co(mal)_3]^{3-}$	14017		113
$[Co(CO_3)_3]^{3-}$	14070	513	93
$[Co(CO_3)_3]^{3-}$	14130		7
$[Co(OH)_2Co(NH_3)_4)_3]^{6+}$, central $\{CoO_6\}$	14850	1710	56
$[Co(OH_2)_6]^{3+}$	15047		113
$[Co(OH_2)_6]^{3+}$	15100		87

TABLE 2c.
Chemical shift: measured from tris(ethylenediamine)cobalt(III) complex cation, σ(2), and line width data.

Complex	σ(2)	Width (Hz)	Lit. No.
$[Co(en)_3]^{3+}$	0	110	42
Λ-*cis*-$[Co((S)\text{-}pn)_3]^{3+}$	82	110	42
Λ-*trans*-$[Co((S)\text{-}pn)_3]^{3+}$	93	96	42
Δ-*cis*-$[Co((S)\text{-}pn)_3]^{3+}$ (mixture)	157	310	42

TABLE 2d.
Chemical shift measured from "aqueous hexanitrocobaltate(III)" solution (ppm).

Complex	σ(3)	Width (Hz)	Lit. No.
$[Co(en)_2(NO_2)_2]^+$, *cis*-	−930		16(+)
$[Co(tn)(gly)(NO_2)_2]$, ab,dc,e,f-	−9.3		58
$[Co(NO_2)_6]^{3-}$ (**)	0		16
$[Co(gly)(NO_2)_4]^{2-}$	130	– –	58
$[Co(NH_3)_2(gly)(NO_2)_2]$, a,b,dc,e,f-	223	– –	58
$[Co(gly)_2(NO_2)_2]^{2-}$, ae,fb,c,d-	455	– –	58
$[Co(NO_2)_6]^{3-}$ (decomp. pr.)	570		16(+)

TABLE 2d (*continued*)

Complex	σ(3)	Width (Hz)	Lit. No.
$[Co(NH_3)_6]^{3+}$	680		16(+)
$[Co(gly)_2(NO_2)_2]^{2-}$, ae,bf,c,d-	781	– –	58
$[Co(gly)_2(NO_2)_2]^{2-}$, ae,cf,b,d-	872	– –	58
$[Co(gly)_2(NO_2)_2]^{2-}$, ae,fc,b,d-	967	– –	58
$[Co(tn)(gly)_2]^+$, ae,bf,cd-	1060	– –	58
$[Co(en)_2CO_3]^+$	1430		16(+)
$[Co(tn)(gly)_2]^+$, ae,bc,df-	1525	– –	58
$[Co(tn)(gly)_2]^+$, ae,fb,cd-	1664	– –	58
$[Co(gly)_3]$, *fac-*	2157	– –	58
$[Co(gly)_3]$, *mer-*	2450	– –	58
$[Co(gly)_2(C_2O_4]^-$, ae,bf,cd-	3128	– –	58
$[Co(gly)_2C_2O_4]^-$, ae,bc,df-	3181	– — –	58
$[Co(gly)_2CO_3]^-$, ae,bf,cd-	3472	– –	58
$[Co(gly)_2CO_3]^-$, ae,bc,df-	3495	– –	58
$[Co(gly)_2C_2O_4]$, ae,fb,cd-	3600	– –	58

(+) The original chemical shift data in reference 16 should be read as one order larger values (as pointed out by Cohen[53]) to explain the spectral charts.

TABLE 2e.
Chemical shift from $[Co(NH_3)_6]^{3+}$ standard (ppm).

Complex	σ(4)	Width (Hz)	Lit. No.
$[Co(CN)_6]^{3-}$	−8100	200	73
$[Co(dmgH)_2CH_3(P(OMe)_3)]$	−6570		49
$[Co(dmgH)_2CH_3(PBu_3)]$	−5530		49
$[Co(dmgH)_2CH_3(CN(Me))]$	−5470		49
$[Co(dmgH)_2CH_3(PPh_3)]$	−5350		49
$[Co(dmgH)_2CH_3(P(p\text{-}C_6H_4OMe)_3)]$	−5340		49
$[Co(dmgH)_2CH_3(AsPh_3)]$	−5200		49
$[Co(dmgH)_2CH_3(SMe_2)]$	−4960		49
$[Co(NH_3)_3(CN)_3]$, *fac-*	−4820	1000	73
$[Co(dmgH)_2CH_3(HIm)]$	−4560		49
$[Co(dmgH)_2CHCl_2(S(Me)_2)]$	−4560		49
$[Co(dmgH)_2Cl(P(OMe)_3)]$	−4550		49
$[Co(dmgH)_2CH_3(NC_5H_5)]$	−4490		49
$[Co(dmgH)_2CH_3(\gamma\text{-pic})]$	−4490		49
$[Co(dmgH)_2CH_3(\beta\text{-pic})]$	−4490		49
$[Co(dmgH)_2CH_3(NMe_3)]$	−4360		49
$[Co(NH_3)_3(CN)_3]$, *mer-*	−4100	2500	73
$[Co(dmgH)_2CH_3(CH_3OH)]$	−4040		49
$[Co(dmgH)_2Cl(P(n\text{-}Bu)_3)]$	−4020		49
$[Co(dmgH)_2Cl(PPh_3)]$	−3360		49
$[Co(NH_3)_4(CN)_2]^+$, *cis-*	−3080	2800	73
$[Co(dmgH)_2Cl(NC_5H_5)]$	−2980		49
$[Co(NH_3)_4(CN)_2]^+$, *trans-*	−2100	4000	73
$[Co(en)(thios)_2]^+$	−2020		101
$[Co(en)_2(NO_2)_2]^+$, *trans-*	−1880	1100	51
$[Co(en)_2(NO_2)_2]^+$, *cis-*	−1700	700	51
$[Co(en)(NH_3)_2(OH)_2]^+$, *cis-,cis-*	−1670	230	39

TABLE 2e (*continued*)

Complex	$\sigma(4)$	Width (Hz)	Lit. No.
$Co(en)(NH_3)_2(OH)_2]^+$, *cis-,trans-*	−1660	560	39
$Co(dien)_2]^{3+}$, dab,cfe- (*mer*)	−1628	450	108
$Co(en)_2NO_2)_2]^+$, *trans-*	−1590	600	73
$Co(en)(NH_3)_2(OH)_2]^+$, *trans-*	−1580	230	39
$Co(en)_2(thios)]^{2+}$	−1510		101
$Co(en)_2(NO_2)_2]^+$, *cis-*	−1510	500	73
$Co(en)_2(NO_2)_2]^+$, *trans-*	−1510	1700	71
$Co(NH_3)_5CN]^{2+}$	−1450	3000	73
$Co(en)(tn)(NO_2)_2]^+$, *trans-*	−1400	1400	71
$Co(en)_2(SO_3)_2]^-$	−1395		101
$Co(en)_2(ThioA\text{-}S)_2]^{3+}$	−1375		101
$Co(en)(NO_2)_4]^-$	−1360	400	73
$Co(NH_3)_2(NO_2)_4]^-$, *trans-*	−1340	1500	73
$Co(dien)(S_2O_3)_3]^{3-}$, *mer-*	−1312	710	108
$Co(dien)(SCN)_3]$, *mer-*	−1276	669	108
$Co(en)(NH_3)_2(NO_2)_2]^+$, *trans-*	−1275	500	51
$Co(en)_2(NH_3)(NO_2)]^{2+}$, *cis-*	−1265	290	51
$Co(en)(NH_3)_2(NO_2)_2]^{2+}$, *c, t-*	−1260	340	51
$Co(en)_2(ThioU\text{-}S)_2]^{3+}$	−1240		101
$Co(dien)_2]^{3+}$, *fac*-(s?,u?)	−1185	358	108
$Co(NH_3)_3(NO_2)_3]$, *mer-*	−1180	800	73
$Co(en)_2(OH)_2]^+$, *cis-*	−1150	230	39
$Co(tn)_2(NO_2)_2]^+$, *trans-*	−1140	1200	73
$Co(tn)_2(NO_2)_2]^+$, *trans-*	−1140	1200	71
$Co(en)_2(S_2O_3)_2]^-$	−1130		101
$Co(en)_2(OH)_2]^+$, *trans-*	−1130	150	39
$Co(en)_3]^{3+}$	−1050		41
$Co(en)_3]^{3+}$	−1030	200	73
$Co(en)_2(ThioS)]^{3+}$	−1025		101
$Co(tn)_2(NO_2)_2]^+$, *cis-*	−1010	1400	73
$Co(tn)_2(NO_2)_2]^+$, *cis-*	−1010	1500	71
$Co(en)_2(ThioA\text{-}N,S)_2]^{3+}$	−998		101
$Co(mbn)_3]^{3+}$, *fac-*	−990	300	62
$Co(benacen)(Me)(NC_5H_5)]$	−980		49
$Co(en)_3]^{3+}$	−980		72
$Co(salen)(Me)]$	−975		21
$Co(mbn)_3]^{3+}$, *mer-*	−965	360	62
$Co(NH_3)_4(NO_2)_2]^+$, *trans-*	−960	280	51
$Co(NH_3)_4(NO_2)_2]^+$, *trans-*	−960	600	73
$Co(l\text{-}pn)_3]^{3+}$, Δ(*fac*)-	−951	100	62
$Co(NH_3)_3(NO_2)_3]$, *fac-*	−950	200	73
$Co(l\text{-}pn)_3]^{3+}$, Δ(*mer*)-	−938	100	62
$Co(en)_2(NO_2)_2]^+$, *cis-*	−930	1200	71
$[Co(en)(NH_3)_3(NO_2)]^{2+}$, *mer-*	−915	280	51
$[Co(en)(gly)(NO_2)_2]$, *cis*(NO_2), *trans*(NH_2)-	−900	7000	71
$[Co(en)(NH_3)_3(NO_2)]^{2+}$, *fac-*	−895	170	51
$[Co(NH_3)_4(NO_2)_2]^+$, *cis-*	−895	150	51
$[Co(dien)(OH)(NO_2)_2]$, *mer-*	−892	382	108
$[Co(NH_3)_4(NO_2)_2]^+$, *cis-*	−890	400	73
$[Co(l\text{-}pn)_3]^{3+}$, Λ(*mer*)-	−863	140	62
$[Co(l\text{-}pn)_3]^{3+}$, Λ(*fac*)-	−859	140	62

TABLE 2e (*continued*)

Complex	σ(4)	Width (Hz)	Lit. No.
$[Co(en)_2(ThioU{-}N,S)_2]^{3+}$	−830		101
$[Co(NH_3)(L\text{-}ala)(NO_2)_3]^-$, *mer*-	−825	3400	71
$[Co(NH_3)(L\text{-}abu)(NO_2)_3]^-$, *mer*-	−820	4200	71
$[Co(NH_3)(L\text{-}nva)(NO_2)_3]^-$, *mer*-	−790	5400	71
$[Co(dien)(NCS)_3]$, *mer*-	−783		108
$[Co(NH_3)(L\text{-}val)(NO_2)_3]^-$, *mer*-	−780	5000	71
$[Co(en)_2(NH_3)_2]^{3+}$, *trans*-	−760	430	51
$[Co(NH_3)(gly)(NO_2)_3]^-$, *mer*-	−760	3300	71
$[Co(benacen)(Me)]$	−730		49
$[Co(tn)(gly)(NO_2)_2]$, *cis*(NO_2), *trans*(NH_2)-	−720	7000	71
$[Co(en)_2(NH_3)_2]^{3+}$, *cis*-	−710	270	51
$[Co(NO_2)_6]^{3-}$ (**)	−710	200	73
$[Co(en)(\beta\text{-}ala)(NO_2)_2]$, *cis*($NO_2$), *trans*($NH_2$)-	−690	8000	71
$[Co(dien)(NH_3)_3]^{3+}$, *fac*-	−650	167	108
$[Co(ibn)_3]^{3+}$, *mer*-	−644	600	62
$[Co(en)(NH_3)_3OH]^{2+}$, *mer*-	−635	430	39
$[Co(ibn)_3]^{3+}$, *fac*-	−626	380	62
$[Co(NH_3)_4(SO_3)_2]^-$	−615		101
$[Co(dien)(NH_3)_3]^{3+}$, *mer*-	−611	430	108
$[Co(en)_2(acetamide)^2]^{3+}$	−598		101
$[Co(salen)Br(PPh_3)]$	−590		21
$[Co(en)_2(ThioA{-}N)_2]^{3+}$	−585		101
$[Co(gly)(NO_2)_4]^{2-}$	−580	1600	71
$[Co(en)(NH_3)_3(OH)]^{2+}$, *fac*-	−560	180	39
$[Co(dien)(NCS)_3]$, *fac*-	−542		108
$[Co(NH_3)_5NO_2]^{2+}$	−530	300	73
$[Co(en)_2(NCS)_2]^+$	−526		101
$[Co(NH_3)_5NO_2]^{2+}$	−525	150	51
$[Co(en)_2(ThioU{-}N)_2]^{3+}$	−520		101
$[Co(NH_3)_2(L\text{-}ala)(NO_2)_2]$, *cis*($NO_2$), *trans*($NH_2,NH_3$)-	−515	3000	71
$[Co(NH_3)_2(L\text{-}abu)(NO_2)_2]$, *cis*($NO_2$), *trans*($NH_2,NH_3$)-	−510	3200	71
$[Co(en)_2(urea)_2]^{3+}$	−501		101
$[Co(NH_3)_4(S_2O_3)_2]^-$	−475		101
$[Co(NH_3)_2(gly)(NO_2)_2]$, *cis*($NO_2$), *trans*($NH_2,NH_3$)-	−455	3600	71
$[Co(NH_3)_2(L\text{-}ala)(NO_2)_2]$, *trans*($NO_2$), *cis*($NH_2,NH_3$)-	−440	3000	71
$[Co(NH_3)_2(L\text{-}abu)(NO_2)_2]$, *trans*($NO_2$), *cis*($NH_2,NH_3$)-	−410	3300	71
$[Co(NH_3)_2(gly)(NO_2)_2]$, *trans*($NO_2$), *cis*($NH_2,NH_3$)-	−385	4200	71
$[Co(tn)(\beta\text{-}ala)(NO_2)_2]$, *cis*($NO_2$), *trans*($NH_2$)-	−380	15000	71
$[Co(en)(NH_3)_4)]^{3+}$	−360	230	51
$[Co(en)_2(gly)]^{2+}$	−350		72
$[Co(L\text{-}ala)_2(NO_2)_2]^-$, *cis*($NO_2$), *trans*($NH_2$)-	−275	4000	71
$[Co(en)_2(NH_3)(N_3)]^+$	−255	700	51
$[Co(L\text{-}val)_2(NO_2)_2]^-$, *cis*($NO_2$), *trans*($NH_2$)-	−248	11000	71
$[Co(aibu)_2(NO_2)_2]^-$, *cis*(NO_2), *trans*(NH_2)-	−243	10000	71
$[Co(L\text{-}abu)_2(NO_2)_2]^-$, *cis*($NO_2$), *trans*($NH_2$)-	−240	10000	71
$[Co(L\text{-}leu)_2(NO_2)_2]^-$, *cis*($NO_2$), *trans*($NH_2$)-	−232	13000	71
$[Co(\beta\text{-}ala)(NO_2)_4]^{2-}$	−230	3000	71
$[Co(L\text{-}nva)_2(NO_2)_2]^-$, *cis*($NO_2$), *trans*($NH_2$)-	−225	10000	71
$[Co(L\text{-}ileu)_2(NO_2)_2]^-$, *cis*($NO_2$), *trans*($NH_2$)-	−220	14000	71
$[Co(en)_2(NH_3)OH]^{2+}$, *cis*-	−220	290	39
$[Co(dien)(en)(OH)]^{2+}$ (*), *fac*-	−192	286	108

TABLE 2e (*continued*)

Complex	σ(4)	Width (Hz)	Lit. No.
$[Co(L\text{-}nleu)_2(NO_2)_2]^-$, *cis*$(NO_2)$, *trans*$(NH_2)$-	−180	14000	71
$[Co(gly)_2(NO_2)_2]^-$, *cis*(NO_2), *trans*(NH_2)-	−170	3500	71
$[Co(dien)(OH)(SCN)_2]$, *mer*-	−162		108
$[Co(dien)(OH)(NCS)_2]$, *mer*-	−129		108
$[Co(dien)(en)(en)(OH)]^{2+}$, *mer*-	−120	588	108
$[Co(en)_2(NH_3)OH]^{2+}$, *trans*-	−110	180	39
$[Co(en)_2(NH_3)Br]^{2+}$, *cis*-	−110	2000	51
$[Co(en)_2(NH_3)Cl]^{2+}$, *cis*-	−100	2500	51
$[Co(NH_3)_5(SCN)]^{2+}$	−68		101
$[Co(NH_3)_4((\pm)\text{-}ptn)_3]^{3+}$	−39.5	196	91
$[Co(\Delta(R,R)\text{-}ptn]^{3+}$	−34.8	197	91
$[Co(L\text{-}ala)(NO_2)_4]^-$· *cis,cis,cis*-	−30	1200	71
$[Co(NH_3)_6]^{3+}$	0	50	51
$[Co(NH_3)_6]^{3+}$	0	200	73
$[Co(dien)(en)(OH)]^{2+}$(**), *fac*-	18	311	108
$[Co(NH_3)_4(meso\text{-}ptn)]^{3+}$	18.2	160	91
$[Co(NH_3)_4)(bdn)]^{3+}$	21.2	144	91
$[Co(NH_3)_4(tn)]^{3+}$	28.2	184	91
$[Co(en)_2(OH_2)ThioU)]^{3+}$	30		101
$[Co(L\text{-}ala)_2(NO_2)_2]^-$, *trans*$(NO_2)$,*cis*$(NH_2)$-	60	1000	71
$[Co(gly)_2(NO_2)_2]^-$, *cis,cis,cis*-	74	1000	71
$[Co(\Lambda(R,R)\text{-}ptn)_3]^{3+}$	85.8	124	91
$[Co(en)(NH_3)_3(N_3)]^{2+}$, *fac*-	90	370	51
$[Co(en)_2(NH_3)(OH_2)]^{3+}$, *trans*-	100		51
$[Co(NH_3)_4(mptn)]^{3+}$	100.3	266	91
$[Co(en)_2(NH_3)OH]^{2+}$, *trans*-	110		51
$[Co(en)_2(OH)(acetamide)]^{2+}$, *cis*-	120		101
$[Co(L\text{-}ala)_2(NO_2)_2]^-$, *trans,trans,trans*-	150	6500	71
$[Co(gly)(\beta\text{-}ala)(NO_2)_2]$, *cis*$(NO_2)$, *trans*$(NH_2)$-	−155	5000	71
$[Co(en)_2(OH_2)(NCS)]^{2+}$	160		101
$[Co(tn)_3]^{3+}$	163.9	161	91
$[Co(gly)_2(NO_2)_2]^-$, *trans*(NO_2),*cis*(NH_2)-	177	700	71
$[Co(tn)_3]^{3+}$	180	200	73
$[Co(dien)(OH)(NH_3)_2]^{2+}$, *fac*-	192	220	108
$[Co(en)_2(NH_3)(OH_2)]^{3+}$, *cis*-	200		51
$[Co(NH_3)(L\text{-}ala)_2(NO_2)]$, *cis*(O),*trans*$(NH_2)$-	207	7000	71
$[Co(NH_3)(L\text{-}abu)_2(NO_2)]$, *cis*(O),*trans*$(NH_2)$-	218	8000	71
$[Co(en)_2(NH_3)(OH)]^{2+}$, *cis*-	220		51
$[Co(NH_3)(L\text{-}nva)_2(NO_2)]$, *cis*(O),*trans*$(NH_2)$-	220	10000	71
$[Co(NH_3)(L\text{-}nleu)_2(NO_2)]$, *cis*(O),*trans*$(NH_2)$-	224	12000	71
$[Co(en)_2(OH_2)(urea)]^{3+}$, *cis*-	224		101
$[Co(en)(NH_3)_3Br]^{2+}$, (*mer,fac*)	240	2500	51
$[Co(en)_2(OH)(acetamide)]^{2+}$, *trans*-	248		101
$[Co(en)_2N_3)_2]^+$, *cis*-	250	500	51
$[Co(dien)(OH)(NH_3)_2]^{2+}$, *mer*-	254	387	108
$[Co(gly)_2(NO_2)_2]^-$, *trans,trans,trans*-	257	6000	71
$[Co(en)(NH_3)_3Cl]^{2+}$, (*mer,fac*)	270	2500	51
$[Co(NH_3)(L\text{-}ileu)_2(NO_2)]$, *cis*(O),*trans*$(NH_2)$-	280	10000	71
$[Co(NH_3(gly)(NO_2)]$, *cis*(O),*trans*(NH_2)-	283	3000	71
$[Co(dien)(OH)(NCO)_2]$, *fac*-	295	270	108
$[Co(\beta\text{-}abu)_2)(NO_2)_2]^-$, *cis*$(NO_2)$,*trans*$(NH_2)$-	297	12000	71

TABLE 2e (*continued*)

Complex	σ(4)	Width (Hz)	Lit. No.
$[\mathrm{Co}(\beta\text{-aibu})_2(\mathrm{NO}_2)_2]^-$, *cis*($\mathrm{NO}_2$),*trans*($\mathrm{NH}_2$)-	298	12000	71
$[\mathrm{Co}(\mathrm{NH}_3)_5\mathrm{NCS}]^{2+}$	352		101
$[\mathrm{Co}(\mathrm{en})_2(\mathrm{OH}_2)(\mathrm{urea})]^{3+}$, *trans*-	375		101
$[\mathrm{Co}(\mathrm{dien})(\mathrm{OH})(\mathrm{NCO})_2]$, *mer*-	375	293	108
$[\mathrm{Co}(\beta\text{-ala})_2(\mathrm{NO}_2)_2]$, *cis*($\mathrm{NO}_2$),*trans*($\mathrm{NH}_2$)-	380	6000	71
$[\mathrm{Co}(\mathrm{dien})(\mathrm{OH})_2(\mathrm{NO}_2)]$, *mer*-	398	669	108
$[\mathrm{Co}(\mathrm{NH}_3)_4(\mathrm{NCS})_2]^+$	420		101
$[\mathrm{Co}(\mathrm{en})_2\mathrm{C}_2\mathrm{O}_4]^+$	460	2000	51
$[\mathrm{Co}(\mathrm{en})(\mathrm{gly})_2]^+$, Cl-*cis*(O)-	520		72
$[\mathrm{Co}(\mathrm{NH}_3)_5(\mathrm{N}_3)]^{2+}$	530	200	51
$[\mathrm{Co}(\mathrm{en})(\mathrm{NH}_3)_3(\mathrm{OH}_2)]^{3+}$, *fac*-	550	8750	51
$[\mathrm{Co}(\mathrm{en})(\mathrm{NH}_3)_3(\mathrm{OH}_2)]^{3+}$, *mer*-	550	14000	51
$[\mathrm{Co}(\mathrm{en})(\mathrm{NH}_3)_3(\mathrm{OH}_2)]^{2+}$, *fac*-	560	315	51
$[\mathrm{Co}(\mathrm{dien})(\mathrm{OH})_2(\mathrm{NO}_2)]$, *fac*-	595		108
$[\mathrm{Co}(\mathrm{en})(\mathrm{NH}_3)_3(\mathrm{OH}_2)]^{2+}$, *mer*-	635	750	51
$[\mathrm{Co}(\mathrm{NH}_3)_5\mathrm{Br}]^{2+}$	670	1000	51
$[\mathrm{Co}(\mathrm{en})(\mathrm{NH}_3)_2(\mathrm{N}_3)_2]^+$	670	600	51
$[\mathrm{Co}(\mathrm{NH}_3)_5\mathrm{Cl}]^{2+}$	700	1000	51
$[\mathrm{Co}(\mathrm{en})_2\mathrm{CO}_3]^+$	730	1900	51
$[\mathrm{Co}(\mathrm{en})_2\mathrm{Br}_2]^+$, *trans*-	810	5500	51
$[\mathrm{Co}(\mathrm{en})_2\mathrm{Br}_2]^+$, *cis*-	810	3000	51
$[\mathrm{Co}(\beta\text{-aibu})_2(\mathrm{NO}_2)_2]^-$, *trans,trans,trans*-	810	10000	71
$[\mathrm{Co}(\mathrm{en})_2\mathrm{Cl}_2]^+$, *cis*-	820	4500	51
$[\mathrm{Co}(\mathrm{tn})(\mathrm{gly})_2]^+$, Cl-*cis*(O)-	820	3500	73
$[\mathrm{Co}(\mathrm{en})_2\mathrm{Cl}_2]^+$, *trans*-	820	8000	51
$[\mathrm{Co}(\mathrm{NH}_3)(\beta\text{-ala})_2(\mathrm{NO}_2)]$, *cis*(O), *trans*($\mathrm{NH}_2$)-	830	9000	71
$[\mathrm{Co}(\mathrm{en})(\mathrm{gly})_2]^+$, *trans*(O)-	860		72
$[\mathrm{Co}(\beta\text{-ala})_2(\mathrm{NO}_2)_2]^-$, *trans,trans,trans*-	896	9000	71
$[\mathrm{Co}(\mathrm{NH}_3)_4(\mathrm{OH})(\mathrm{acetamide})]^{2+}$	901		101
$[\mathrm{Co}(\mathrm{NH}_3)_5(\mathrm{OH}_2)]^{3+}$	930		51
$[\mathrm{Co}(\mathrm{en})_2(\mathrm{OH}_2)_2]^{3+}$, *trans*-	950		51
$[\mathrm{Co}(\mathrm{tn})(\mathrm{gly})_2]^+$, *trans*(O)-	960	12000	73
$[\mathrm{Co}(\mathrm{NH}_3)_4(\mathrm{OH})(\mathrm{urea})]^{2+}$	988		101
$[\mathrm{Co}(\mathrm{NH}_3)_5(\mathrm{OH})]^{2+}$	990	230	51
$[\mathrm{Co}(\mathrm{en})_2(\mathrm{OH}_2)_2]^{3+}$, *cis*-	1000	11370	51
$[\mathrm{Co}(\mathrm{en})_2(\mathrm{OH}_2)_2]^{3+}$, *cis*-	1015		101
$[\mathrm{Co}(\mathrm{NH}_3)_4(\mathrm{N}_3)_2]^+$, *trans*-	1070	300	51
$[\mathrm{Co}(\mathrm{NH}_3)_2(\mathrm{OH}_2)(\mathrm{SO}_3)_2]^-$	1095		101
$[\mathrm{Co}(\mathrm{NH}_3)_4(\mathrm{OH}_2)_2(\mathrm{ThioA})]^{2+}$	1098		101
$[\mathrm{Co}(\mathrm{NH}_3)_4(\mathrm{N}_3)_2]^+$, *cis*-	1110	210	51
$[\mathrm{Co}(\mathrm{NH}_3)_2(\mathrm{OH}_2)_2(\mathrm{ThioU})]^{2+}$	1115		101
$[\mathrm{Co}(\mathrm{NH}_3)_4(\mathrm{OH}_2)(\mathrm{NCS})]^{2+}$	1120		101
$[\mathrm{Co}(\mathrm{en})_2(\mathrm{OH})_2]^+$, *trans*-	1130	260	51
$[\mathrm{Co}(\mathrm{en})_2(\mathrm{OH})_2]^+$, *cis*-	1150	400	51
$[\mathrm{Co}(\mathrm{en})(\mathrm{NH}_3)_2\mathrm{Cl}_2]^+$, *trans*-	1150	4000	51
$[\mathrm{Co}(\mathrm{en})(\mathrm{NH}_3)_2\mathrm{Br}_2]^+$, *trans*-	1160	4800	51
$[\mathrm{Co}(\mathrm{en})(\mathrm{NH}_3)_2\mathrm{Cl}_2]^+$, *cis, trans*-	1170	3000	51
$[\mathrm{Co}(\mathrm{dien})(\mathrm{OH})_2(\mathrm{SCN})]$, *mer*-	1178		108
$[\mathrm{Co}(\mathrm{en})(\mathrm{NH}_3)_2(\mathrm{CO}_3)]^+$	1180	1900	51
$[\mathrm{Co}(\mathrm{en})_2(\mathrm{OH})_2]^+$, *cis*-	1183		101
$[\mathrm{Co}(\mathrm{dien})(\mathrm{OH})_2(\mathrm{NCO})]$, *fac*-	1198	192	108
$[\mathrm{Co}(\mathrm{dien})(\mathrm{OH})_2(\mathrm{urea\text{-}N})]^+$, *mer*-	1200	958	108

TABLE 2e (*continued*)

Complex	σ(4)	Width (Hz)	Lit. No.
$[Co(en)_2(OH)_2]^+$, *trans-*	1213		101
$[Co(dien)(OH)_2(NCO)]$, *mer-*	1225	297	108
$[Co(dien)(OH)_2NH_3]^+$, *mer-*	1285	239	108
$[Co(dien)(OH)_2en]^+$	1330	1916	108
$[Co(dien)(OH)_2(urea\text{-}N)]^+$, *fac-*	1335	575	108
$[Co(gly)_3]$, *fac-*	1410	2500	73
$[Co(gly)_3]$, *fac-*	1410		72
$[Co(L\text{-}ala)_3]$, *mer-*	1460	6500	71
$[Co(NH_3)_4CO_3]^+$	1580	1100	51
$[Co(en)(NH_3)_2(OH)_2]^+$, *trans-*	1580	400	51
$[Co(L\text{-}nva)_3]$, *mer-*	1600	7000	71
$[Co(dien)(OH_2)_2Cl]^{2+}$, *mer-*	1612	536	108
$[Co(dien)(OH_2)_2Cl]^{2+}$, *fac-*	1651	395	108
$[Co(NH_3)_4Cl_2]^+$, *trans-*	1660	4000	51
$[Co(NH_3)_4Cl_2]^+$, *cis-*	1660	2000	51
$[Co(en)(NH_3)_2(OH)_2]^+$, *cis, trans-*	1660	1030	51
$[Co(en)(NH_3)_2(OH)_2]^+$, *cis,cis-*	1670	400	51
$[Co(dien)(urea\text{-}O)_3]^{3+}$, *mer-*	1712	730	108
$Co(gly)_3]$, *mer-*	1730	6000	71
$Co(gly)_3]$, *mer-*	1740	6500	73
$Co(gly)_3]$, *mer-*	1740		72
$Co(NH_3)_3(N_3)_3]$, *mer-*	1750	710	51
$Co(dien)(OH_2)_3]^{3+}$, *mer-*	1782	383	108
$Co(NH_3)_4(OH_2)_2]^{3+}$, *cis-*	1880		101
$Co(NH_3)_4(OHF_{32})_2]^{3+}$, *cis-*	1810	5250	51
$Co(NH_3)_3(N_3)_3]$, *fac-*	1820	170	51
$Co(NH_3)_4(C_2O_4)]^+$	1850		51
$Co(dien)(urea\text{-}O)_3]^{3+}$, *fac-*	1882	580	108
$Co(NH_3)_4(OH_2)]^+$, *cis-*	1940	245	51
$Co(NH_3)_4(OH)_2]^+$, *cis-*	1987		101
$Co(NH_3)(OH_2)_3(SO_3)_2]^-$	2200		101
$Co(NH_3)(OH_2)_3(ThioA)]^{3+}$	2210		101
$Co(en)(C_2O_4)_2]^-$	2250	3200	51
$Co(NH_3)(OH_2)_3(ThioU)_2]^{3+}$	2260		101
$Co(dien)(OH_3)]$, *mer-*	2265		108
$Co(NH_3)(OH_2)_3(ThioS)]^{3+}$	2272		101
$Co(gly)_2(C_2O_4)]^-$, C1-*cis*(N)-	2420	3700	73
$Co(gly)_2(C_2O_4)]^-$, C1-*cis*(N)-	2420		72
$Co(gly)_2(C_2O_4)]^-$, C2-*cis*(N)-	2470		72
$Co(gly)_2(C_2O_4)]^-$, C2-*cis*(N)-	2470	4000	73
$Co(\beta\text{-}ala)_3]$, *mer-*	2500	8000	71
$Co(ThioS)_3]^{3+}$	2578		101
$Co(NH_3)_3(OH_2)_3]^{3+}$, *fac-*	2630	350	51
$Co(en)(NH_3)(OH)_3]$, *fac-*	2710	350	51
$Co(NH_3)_2(C_2O_4)_2]^-$	2780	1500	51
$Co(OH_2)_4(SO_3)_2]^{2-}$	2898		101
$Co(OH_2)_4(ThioU)_2]^{3+}$	2908		101
$Co(gly)(C_2O_4)]^-$, *trans*(N)-	2920	12500	73
$Co(gly)_2(C_2O_4)]$, *trans*(N)-	2920		72
$Co(en)(CO_3)_2]^-$	2940	2400	51
$Co(OH_2)_4(ThioU)_2]^{3+}$	2968		101
$Co(OH_2)_4(ThioS)_2]^{3+}$	2975		101

TABLE 2e (*continued*)

Complex	σ(4)	Width (Hz)	Lit. No.
$[Co(NH_3)_2(CO_3)_2]^-$	3550	1600	51
$[Co(gly)(C_2O_4)_2]^{2-}$	3680	4600	73
$[Co(gly)(C_2O_4)_2]^{2-}$	3680		72
$[Co(C_2O_4)_3]^{3-}$	4700	250	51
$[Co(C_2O_4)_3]^{3-}$	4800		72
$[Co(C_2O_4)_3]^{3-}$	4800	200	73
$[Co(CO_3)_3]^{3-}$	5770	250	51

TABLE 2f.
Cobalt-59 chemical shift from tris(acetylacetonato)cobalt(III)/Chloroform (ppm).

Complex	σ(5)	Width (Hz)	Lit. No.
[Co(acac)$_3$Nd(dpm)$_3$]	−417	400	79,92
[Co(acac)$_3$Pr(dpm)$_3$]	−416	450	79,92
[Co(acac)$_3$Nd(fod)$_3$]	−396	76	79,92
[Co(acac)$_3$Pr(fod)$_3$]	−394	126	79,92
[Co(acac)$_3$Sm(dpm)$_3$]	−378	875	79,92
[Co(acac)$_3$Sm(fod)$_3$]	−344	50	79,92
[Co(acac)$_3$La(dpm)$_3$]	−332	680	79,92
[Co(acac)$_3$La(fod)$_3$]	−281	202	79,92
[Co(acac)$_3$Eu(fod)$_3$]	−257	50	79,92
[Co(acac)$_3$Eu(fod)$_3$]	−252	600	79,92
Δ-*c*-[Co((−)-hmcar)$_3$]	−128	314	42
Λ-*c*-[Co((+)-hmcar)$_3$]	−128	314	42
Λ-*c*-[Co((−)-hmcar)$_3$]	−99	620	42
Δ-*c*-[Co((+)-hmcar)$_3$]	−99	620	42
Δ-*t*-[Co((+)-hmcar)$_3$]	−90	730	42
Λ-*t*-[Co((−)-hmcar)$_3$]	−90	730	42
Δ-*t*-[Co((−)-hmcar)$_3$]	−68	710	42
Λ-*t*-[Co((+)-hmcar)$_3$]	−68	710	42
[Co(ppd)$_3$], *cis*-	−59	130	42
[Co(ppd)$_3$], *trans*-	−59	320	42
[Co(acac)$_3$]	0	120	42
[Co(bzac)$_3$], *trans*-	12	270	42
[Co(bzac)$_3$], *cis*-	50	250	42
[Co(tfac)$_3$], *cis*-	76	160	42
[Co(tfac)$_3$], *trans*-	80	190	42
Λ-*t*-[Co((+)-atc)$_3$]	284	270	42
Δ-*t*-[Co((+)-atc)$_3$]	289	310	42
[Co(TTA)$_3$]	295	250	42
Λ-*c*-[Co((+)-atc)$_3$]	304	290	42
Δ-*c*-[Co((+)-atc)$_3$]	356	220	42

Almost all cobalt complexes are mononuclear, but several binuclear or oligonuclear complexes such as carbonyls and dithiocarbamates are also studied thoroughly, but the assignments of these signals for the site of these moieties have not been sufficiently described. For such a case, each component of the multiplet spectra are denoted by Roman numbers from the smaller chemical shift side.

(*) These signals seem to be assigned to acontaminants occasionally co-existing in these complexes (for stance, $[Co(en)_3]^{3+}$). These acontaminants usually show much sharper signals which are more readily served than the main components.

(**) The species existing in aqueous sodium hexanitrocobaltate(III) solution is not hexakis(nitrito-N)-baltate(III). see Ref. 127.

(***) The stereochemical notation of dien and tetraen complexes in the Reference 93, 94, and 95 are not nsistent with each other, and seems to contain some proof-reading errors. The original descriptions are plied in this table.

TABLE 3

Chemical shift σ(1), and line width data for cobalt-59 of lower oxidation states and organometallics.

omplex	σ(1)	Width (Hz)	Lit. No.
$Co(PF_3)_4]^-$ /water	−4220	narrow	18
$o(PF_3)_4H$ /C_7H_{16}	−3910	3840	18
$o(CO)_4H$ /C_5H_{12}	−3721	3240	18
$Co(CO)_4]^-$ /water	−3100	narrow	18
$Co(CO)_4$-$Mn(CO)_5$	−2900		36
$HRuCO_3(CO)_{12}$(minor peak)	−2768		117
$HRuCO_3(CO)_{10}(P(Ph)_3)_2$ /CD_2Cl_2 [intensity 2]	−2715		117
$HRuCO_3(CO)_{11}(P(Ph)_3)$ /CD_2Cl_2 (minor peak)	−2712		117
$Co(C_5H_5)(CO)_2$ /C_6H_6	−2675	6800	18
$Co(C_5H_5)(CO)_2$ /C_7H_{16}	−2675	6780	18
$HRuCo_3(CO)_{11}(N(Me)_3)$ /CD_2Cl_2	−2649		117
$HRuCo_3(CO)_{10}$(TMEDA) /CD_2Cl_2	−2649		117
$HRuCo_3(CO)_{11}(P(Ph)_3)$ /CD_2Cl_2 [intensity 2]	−2648		117
$HRuCo_3(CO)_{12}$ /CD_2Cl_2	−2648		117
$HRuCO_3(CO)_{11}(P(Ph)_3)$ /CD_2Cl_2 (minor peak)	−2641		117
$HRuCO_3(CO)_{11}(N(Et)_3)$ /CD_2Cl_2	−2630		117
$HRuCO_3(CO)_{10}(P(Ph)_3)_2$ /CD_2Cl_2 [intensity 1]	−2575		117
$HRuCO_3(CO)_{11}(P(Ph)_3)$ /CD_2Cl_2 [intensity 1]	−2574		117
$HRuCO_3(CO)_{10}(P(Ph)_3)_2$ /CD_2Cl_2 (minor peak)	−2530		117
$HgCo_2(CO)_8$ /C_6H_6	−2520	22860	18
$HRuCo_3(CO)_{12}$ /CD_2Cl_2 (minor peak)	−2514		117
$HRuCo_3(CO)_{12}$ /CD_2Cl_2 (minor peak)	−2464		117
$Co(C_5H_5)_2]^+$ (Cl-, 10% in MeOH)	−2410	21600	18
$Co(C_5H_5)_2]^+$ /water	−2410	14600	18
$Co(C_5H_5)_2]^+$ (Cl-, 4% in MeOH)	−2410	13600	18
$Co(C_5H_5)_2]^+$	−2200		26
$Co_2(CO)_8$ /C_5H_{12}	−2101	6350	18
$Co_2(CO)_8$ /C_6H_6	−2101	10410	18
$Co_4(CO)_{12}$ /$CDCl_3$ [I] (basal)	−2065	12000	109
$Co_4(CO)_{12}$ /C_5H_{12} [I] (basal)	−1961		18
$Co(C_5H_5)(C_6H_8)$ /toluene-d_8	−1820	13000	110
$Co(C_5H_5)(C_6H_4(CF_3)_4)$ /toluene-d_8	−1726	14400	110
$Co(C_5H_5)(C_5H_5$-$CF_3)$ /C_6D_6	−1640	16800	110
$Co(C_5H_5(C_5H_5$-Me) /C_6D_6	−1627	16800	110
$Co(C_5H_5)(C_4H_6)$ /C_6D_6	−1625	8100	110
$Co(C_5H_5)(C_4H_6)$ /THF-d_8	−1620	8650	110
$Co(C_5H_5)(C_4H_5$-$C_2H_4CN)$ /C_6D_6	−1601	14400	110
$Co(C_5H_5)(C_4H_5$-$C_3H_7)$ /C_6D_6	−1571	10200	110
$Co(C_5H_5)(C_4H_5$-$C_2H_4C_3H_5)$ /C_6D_6	−1567	10400	110
$Co(C_5H_5)(C_5H_5$-CH_2-$C_3H_5)$ /C_6D_6	−1560	18750	110
$Co(C_2H_4)_2(C_5Me)_5)$ /toluene-d_8	−1470	9900	110
Co(indenyl)(C_6H_8) /THF-d_8	−1443	11600	110

TABLE 3 (*continued*)

Complex	σ(1)	Width (Hz)	Lit. No.
$\mathrm{Co(C_5H_5)(C_5H_6)}$ /$\mathrm{C_6D_6}$	−1439	9600	110
$\mathrm{Co(COD)(C_5(Me)_5)}$ /toluene-$\mathrm{d_8}$	−1413		102
$\mathrm{Co(C_5H_5)(CHD)}$ /toluene-$\mathrm{d_8}$	−1400	10100	110
$\mathrm{Co(CO)_3NO}$ /$\mathrm{C_7H_{16}}$	−1365	546	18
$\mathrm{Co(C_5H_5)(CHT)}$ /THF-$\mathrm{d_8}$	−1319	10500	110
$\mathrm{Co(C_5H_5(benzo\text{-}CHT)}$ /toluene-$\mathrm{d_8}$	−1319	20000	110
$\mathrm{Co(\pi\text{-}(2\text{-}Me)C_3H_4)}$ /THF-$\mathrm{d_8}$	−1306	13000	110
$\mathrm{Co(C_2H_4)_2(C_5H_4Me)}$ /toluene-$\mathrm{d_8}$	−1294	7350	110
$\mathrm{Co(COD)(C_5H_3(CH_2)_3)}$ /toluene-$\mathrm{d_8}$	−1284	8400	110
$\mathrm{Co(C_5H_4\text{-}Si(Me)_3)(CHD)}$ /toluene-$\mathrm{d_8}$	−1282	13200	110
$\mathrm{Co(indenyl)(C_6H_4(Me)_4)}$ /toluene-$\mathrm{d_8}$	−1275	18000	110
$\mathrm{Co(COD)(C_5H_3(CH_2)_3)}$/toluene-$\mathrm{d_8}$	−1261		102
$\mathrm{Co(C_5H_5)(anthracene)}$ /toluene-$\mathrm{d_8}$	−1243	7600	110
$\mathrm{Co(indenyl)(C_6H_4(CF_3)_4}$ /toluene-$\mathrm{d_8}$	−1236	13000	110
$\mathrm{Co(C_5H_5)(C_2H_4)_2}$ /THF-$\mathrm{d_8}$	−1235	6800	110
$\mathrm{Co(indenyl)(C_4H_6)}$ /$\mathrm{C_6D_6}$	−1234	11200	110
$\mathrm{Co(C_5H_5)(C_2H_4)_2}$ /toluene-$\mathrm{d_8}$	−1231	7000	110
$\mathrm{Co(indenyl)(C_4H_4(CH_3)_2)}$ /toluene-$\mathrm{d_8}$	−1230	12600	110
$\mathrm{Co(C_5H_5)((CH_2)_2C{=}CH_2)_2}$ /$\mathrm{C_6D_6}$	−1229	9300	110
$\mathrm{Co(COD)(C_5H_4CH_3)}$ /toluene-$\mathrm{d_8}$	−1227		102
$\mathrm{Co(C_5H_5)(COD)}$ /toluene-$\mathrm{d_8}$	−1190	9150	110
$\mathrm{Co(C_2H_4)_2(C_5H_4Si(Me)_3)}$ /toluene-$\mathrm{d_8}$	−1187	10200	110
$\mathrm{Co(indenyl)(isoprene)}$ /toluene-$\mathrm{d_8}$	−1180	11400	110
$\mathrm{Co(C_5H_5)(COD)}$ /THF-$\mathrm{d_8}$	−1178	9150	110
$\mathrm{Co(COD)(C_5H_5)}$ /toluene-$\mathrm{d_8}$	−1176		102
$\mathrm{Co(COD)(C_5H_4\text{-}Si(Me)_3)}$ /toluene-$\mathrm{d_8}$	−1170	11100	110
$\mathrm{Co(COD)(C_5H_4C(Me)_3)}$ /toluene-$\mathrm{d_8}$	−1166		102
$\mathrm{Co(COD)(C_5H_4\text{-}Si(Me)_3)}$ /toluene-$\mathrm{d_8}$	−1149		102
$\mathrm{Co(C_5H_5)(1,5\text{-}C_6H_{10})}$ /$\mathrm{C_6D_6}$	−1109	8550	110
$\mathrm{Co(C_5H_5(1,6\text{-}C_7H_{12})}$ /toluene-$\mathrm{d_8}$	−1102	9750	110
$\mathrm{Co(C_5H_5)_2(CH_2CHCN)_2}$ /toluene-$\mathrm{d_8}$	−1089	12400	110
$\mathrm{Co(COD)(C_5H_4\text{-}C_6H_5)}$ /toluene-$\mathrm{d_8}$	−1088		102
$\mathrm{Co(COD)(C_5H_4COCH_3)}$ /toluene-$\mathrm{d_8}$	−1055		102
$\mathrm{Co(C_7H_9)(C_7H_6\text{-}SiMe_3)}$ /toluene-$\mathrm{d_8}$	−1036	12500	110
$\mathrm{Co(C_5H_5)(C_6H_4)(Ph)_4)}$ /toluene-$\mathrm{d_8}$	− 930	18800	110
$\mathrm{Co(indenyl)(CHT)}$ /THF-$\mathrm{d_8}$	− 899	12400	110
$\mathrm{Co(indenyl)(C_2H_4)_2}$ /THF-$\mathrm{d_8}$	− 879	19200	110
$\mathrm{Co(COD)(Me_3Si\text{-}indenyl)}$ /toluene-$\mathrm{d_8}$	− 858	14000	110
$\mathrm{Co(indenyl)(COD)}$ /toluene-$\mathrm{d_8}$	− 851	7700	110
$\mathrm{Co(indenyl)(COD)}$ /THF-$\mathrm{d_8}$	− 849	9450	110
$\mathrm{Co_4(CO)_{12}}$ /$\mathrm{C_5H_{12}}$ [II] (apical)	− 814		18
$\mathrm{Co(\pi\text{-}C_3H_5)_3}$ /THF-$\mathrm{d_8}$	− 796	3750	110
$\mathrm{Co(\pi\text{-}C_3H_5)(C_5H_5)(Me)}$ /$\mathrm{C_6D_6}$	− 788	6600	110
$\mathrm{Co(indenyl)(1,5\text{-}C_6H_{10})}$ /THF-$\mathrm{d_8}$	− 756	9750	110
$\mathrm{Co(indenyl)(1,5\text{-}C_6H_{10})}$ /toluene-$\mathrm{d_8}$	− 747	10500	110
$\mathrm{Co_4(CO)_{12}}$ /$\mathrm{CDCl_3}$	− 715	4000	109
$\mathrm{Co(\pi\text{-}C_3H_4)(C_5H_5)CH_2C_6H_5}$ /$\mathrm{C_6D_6}$	− 455	11000	110
$\mathrm{Co(COD)(\pi\text{-}C_8H_{11})}$ /toluene-$\mathrm{d_8}$	− 275	3700	110
$\mathrm{Co(\pi\text{-}C_3H_4)(C_5H_5)Br}$ /$\mathrm{C_6D_6}$	1050	10000	110

6.3. Stereoisomer Discrimination

The ratio of chemical shift against CFSE is fairly large, and the improvement of NMR spectrometers makes it possible to determine the chemical shift differences in the magnitude of 1.0 ppm accurately for the sharp cobalt-59 NMR spectra. This improvement enables us to apply cobalt-59 NMR to various similar complexes such as diastereomers. The stereochemistry of tris-chelates of cobalt(III) complexes has been extensively studied mainly with the visible-ultraviolet spectroscopy (absorption and circular dichroism). The discrimination of the small differences in similar stereoisomers by electronic spectra is usually very difficult. The 1 ppm chemical shift difference of cobalt-59 corresponds to the difference in the first absorption maxima of 0.03 nm, which is almost impossible to detect as noted above.

Tris(propylenediamine)chelates and several other tris-diammine chelates are well characterized by cobalt-59 NMR.[46,48] Also several diastereotopic isomers of the tris(acetylcamphorato)- and tris(hydroxymethylenecarvonato)-cobalt(III) chelates can be easily discriminated.[42] Seven possible isomers for μ-peroxo bis-((tetraen)-cobalt(III)) complex, $[(Co(tetren)_2O_2]^{4+}$ can also be characterized by cobalt-59 chemical shift data.[93,94]

7. SPIN-SPIN COUPLING

The scalar coupling constants including those of cobalt-59 have been scarcely reported relative to chemical shift data. The quadrupolar relaxation of cobalt-59 causes broadening of the line width and prevented us from determining the exact (splitting by spin–spin couplings.) Although several ^1J(Co–X) values were reported in highly-symmetric complexes, such as tetracarbonylcobaltate(-I)[18] or hexacyanocobaltate(III),[12,13] from the cobalt-59 NMR spectra, the number of the reported coupling constants are relatively small.

The cobalt(III) complexes with small sterically hindered ligands such as trimethyl phosphite or cage phosphite esters show clear scalar coupling with narrow lines.[61,78,125]

The reported spin–spin coupling constants are summarized in Table 5. Several values were also obtained from the NMR spectra of the ligand nuclei, such as carbon-13 or nitrogen-15, occasionally by the use of enriched isotopomers.

Only one $^4J(^{59}$Co–N–C–C–H) was reported for the Schiff-base complex, nitrosyl-bis(o-hydroxyacetophenoneoximato)cobalt(III).[103] Its magnitude (ca. 540 Hz) is surprisingly large, but there is no data to compare with this at present.

8. EFFECT OF PARAMAGNETISM

Almost all complexes containing tervalent cobalt are diamagnetic except the well-known hexafluorocobaltate(III) and several rather peculiar ones such as heteropolymolybdates. These essentially paramagnetic complexes are impossible to measure using the cobalt-59 NMR spectra, although some spin cross-over complexes have been investigated by Navon and his groups.[87,106]

Spin cross-over complexes have been studied by cobalt-59 NMR spectroscopy. The temperature dependence of the chemical shift of hexaaquacobalt(III) cation[87] and the typical spin-crossover complex of trinuclear bis(cyclopentadienylcobalttris(diethylphosphonato))cobalt(III)[106] are fairly large, and the contribution of paramagnetism can be easily analyzed.

TABLE 4a.
Ligand Shift Parameter $\delta_i(L)$.[51]

Ligand	first (ppm)	second (ppm)	third (ppm)
NO_2^-	−530 ± 20	−420 ± 100	—
N_3^-	480 ± 50	40 ± 50	660 ± 50
Cl^-	650 ± 50	900 ± 50	
Br^-	620 ± 50	900 ± 50	
OH^-	950 ± 100	950 ± 100	1100 ± 100
H_2O	900 ± 100	870 ± 100	830 ± 100

Ligand	second (ppm)	fourth (ppm)	sixth (ppm)
$C_2O_4^{2-}$	1200 ± 100	1500 ± 100	2000
CO_3^{2-}	1500 ± 100	1900 ± 100	2200

TABLE 4b.
Chemical shift (S_L) and line broadening (γ_L) parameters for cobalt(III) complexes.[93]

Ligand	$S_L(10^{-5}\ ppm^{-1})$	$\gamma_L(Hz^{1/2})$	f
$\underline{C}N^-$	4.446	79.500	1.7
$\underline{N}(CH_2CH_2NH_2)_3$	3.087	65.958	
$\underline{N}H(CH_2CH_2NH_2)_2$ (fac)	2.895	59.985	1.29
$\underline{N}H_2CH$-	2.858	59.210	1.30
$NH(CH_2CH_2\underline{N}H_2)_2$ (mer)	2.823	58.488	1.29
$\underline{N}H_2CH_2CH_2\underline{N}H_2$	2.755	57.080	1.28
$\underline{N}H_3$	2.608	52.000	1.25
$\underline{N}CS^-$	2.476	45.000	1.02
$\underline{S}CN^-$	2.320	38.000	0.73
$\underline{O}_2^{2-}$	2.169	44.446	
$\underline{I}^-$	2.168	41.000	
$\underline{N}_3^-$	2.125	43.000	0.83
$\underline{B}r^-$	2.125	35.938	0.72
$\underline{C}l^-$	2.058	33.895	0.78
$C\underline{O}_3^{2-}$	2.017	35.500	
$\underline{O}\underline{H}^-$	1.930	19.659	
$H_2\underline{O}$	1.920	19.613	1.00

The cobalt-59 NMR spectra of the adducts of cobalt(III) complexes with paramagnetic species, such as so-called "lanthanide shift reagents" can be sufficiently recorded by ordinary measurements. Paramagnetic spin delocalization (contact shift) and dipolar effect (pseudocontact shift) were estimated by Hirayama and his coworkers,[79,92] on the 1:1 adducts of the tris(dipivaloylmethanato)- and tris(heptafluorodimethyloctanedionato)- chelates of lanthanides(III) with tris(acetylacetonato)-cobalt(III) in several organic solvents such as chloroform. The chemical shift change for the paramagnetic complexes seems not as large as expected. The iamagnetic adducts with lanthanum chelates show a relatively large shift, (so-called FS, complex formation shift), but the paramagnetic contribution to the chemical hift seems much smaller in this case. These paramagnetic shifts were interpreted with oth the contact shift and pseudocontact shift terms. The line width shows wide hanges for these paramagnetic chelates. The reason is as yet unclear.

. ORGANOMETALLICS

xcept for a small number of highly symmetric moieties such as tetracarbonylobaltate(-I) and nitrosyltricaronylcobalt,[18] almost all organocobalt species show elatively large line widths and it is very hard to measure exactly the cobalt-59 MR spectra.

Characterization of the cobalt carbonyl species in solution has been carried out y several groups.[16,18,53,109] The characterization of diamagnetic cobalt entities in hese organocobalt(III) complexes seems to be highly improved by the introduction f high-field NMR. Several phosphine- or phosphite derivatives and heteronuclear arbonyls have also been investigated.[53,114,117]

Alkylcobalt(III) complexes with dimethylglyoximato- or other Schiff-base ligands ave been studied by various research groups[45,49,85] who are interested in the ioinorganic activities similar to the Vitamin B_{12}.

A German research group found the existence of excellent correlation between obalt-59 chemical shift and catalytic activities in the alkylation reaction. Their ecent report[102] included the observation that chemical shifts of cyclooctadieneobalt(I) complexes clearly correlate with the catalytic activities for the formation of yridine derivatives from alkynes and nitriles. Chemical shift and line width data for rganocobalt complexes and some complexes of the lower oxidation states are shown n Table 3.

10. MEDIUM EFFECTS, CHARACTERIZATION OF SOLVENTS

It is possible to determine accurately the slight changes in the electronic states of the obalt nucleus by cobalt-59 NMR as noted before. This high sensitivity has been successfully applied to several interesting physicochemicals in solution.

Preferential solvation has been studied in several binary solvent mixtures. From the chemical shift change of tris(acetylacetonato)cobalt(III),[7,28,123] much precise information can be deduced that could not be found from the use of other spectroscopic methods such as proton or carbon-13 magnetic resonance and visible-ultraviolet spectroscopy.

The isotopic composition of the solvent is also expected to affect the chemical shifts of cobalt complexes in solution. The change in surroundings (secondary coordination sphere) can be detected effectively, and applied to the determination of the isotopic composition of many protic solvents. The successive substitution of amine protons by solvent deuterons for tris(ethylenediamine)cobalt(III) complex cation was traced firstly by Sudmeier[38] and more extensively by Doddrell[68] and Harris.[104] The usage of the cobalt-59 spectral change of hexaamminecobalt(III) cations was proposed as the indicator of the isotopic composition of water-heavy water mixture.[99,100,107] The hexacyanocobaltate(III) complex was also applied to study the change of surroundings[81,84,90] including isotopic composition.

TABLE 5
Spin–spin coupling constants including cobalt-59.

Complex	Coupling	J(Hz)	Observed Nuclei	Ref.
$[Co(CN)_6]^{3-}$	$^1J(Co\text{-}^{13}C)$	126	^{59}Co	12
$[Co(CN)_6]^{3-}$	$^1J(Co\text{-}^{13}C)$	126	^{59}Co	13
$[Co(CN)_6]^{3-}$	$^1J(Co\text{-}^{13}C)$	125	^{13}C	129
$[Co(CO)_4]^-$	$^1J(Co\text{-}^{13}C)$	287	^{59}Co	18
$[Co(NH_3)_6]^{3+}$	$^1J(Co\text{-}^{14}N)$	40.8	^{59}Co	76
$[Co(NO_2)_6]^{3-}$	$^1J(Co\text{-}^{14}N)$	46	^{59}Co	76
$[Co(en)_3]^{3+}$	$^1J(Co\text{-}^{14}N)$	50	^{59}Co	77
$[Co(^{15}NH_3)_6]^{3+}$	$^1J(Co\text{-}^{15}N)$	63	^{59}Co	68
$[Co(^{15}NO)(ketox)_2]$	$^1J(Co\text{-}^{15}N)$	9	^{15}N	121
$[Co(^{15}NO_2)_5OH_2]^{2-}$	$^1J(Co\text{-}^{15}N)$	70	^{59}Co	127
$[Co(NH_3)_5(^{15}NH_3)]^{3+}$	$^1J(Co\text{-}^{15}N)$	62.5	^{15}N	130
$[Co(en\text{-}^{15}N, {}^{15}N)_3]^{3+}$	$^1J(Co\text{-}^{15}N)$	63.8	^{15}N	130
$[Co(P((OCH_2)_3CCH_3)_6]^{3+}$	$^1J(Co\text{-}^{31}P)$	412	^{59}Co	78
$[Co(P(OCH_3)_3)_6]^{3+}$	$^1J(Co\text{-}^{31}P)$	414	^{59}Co	61
$[Co(P(OCH_3)_3)_6]^{3+}$	$^1J(Co\text{-}^{31}P)$	443	^{59}Co	78
$[Co(PF_3)_4]^-$	$^1J(Co\text{-}^{31}P)$	1222	^{59}Co	18
$[Co(CN)_6]^{3-}$	$^2J(Co\text{–}C\text{-}^{15}N)$	3.3	^{59}Co	12
$[Co(^{15}NH_3)_6]^{3+}$	$^2J(Co\text{–}N\text{-}^{1}H)$	5	^{59}Co	68
$[Co(PF_3)_4]^-$	$^2J(Co\text{-}P\text{-}^{19}F)$	56	^{59}Co	18
$[Co(^{15}NO)(ketox)_2]$	$^4J(Co\text{–}N\text{–}C\text{–}C\text{-}^{1}H)$	540	^{59}Co	121

The high sensitivity of the cobalt-59 chemical shift has been applied to the determination of the effect of the interaction of surrounding solvent molecules. Even the different isotopic compositions of the solvent water shows the remarkable characteristic differences of the spectral feature of cobalt complexes.[81,104] It is very surprising that the change of isotopic composition (proton–deuteron) can be detected using cobalt-59 NMR in spite of the lack of direct chemical bonding.

Mayer and his co-workers found that there is good correlation between the cobalt-59 chemical shift of tris(ethylenediamine)cobalt(III) trifluoromethanesulfonate and "acceptor numbers" of various solvents.[70,74,98] Acceptor numbers are originally defined from the chemical shift change of phosphorus-31 in trimethylphosphine oxide in various solvents. Therefore, the parallelism of the cobalt-59 and phosphorus-31 chemical shifts might have been expected, but the wide range of cobalt-59 NMR chemical shifts seems to give us much information on the various solvents. Only the limited solubility of cobalt complexes seems to be the severe weakpoint.

Line widths show clear dependence on the "donor numbers" of solvents. From the zero-field extrapolation, the limited line widths of several cobalt(III)complexes show positive correlation with these donor numbers.[94]

Association of cobalt(III) complexes with biological macromolecules can be studied by cobalt-59 NMR.[83,120] The line broadening gives us information on the secondary coordination sphere, and the affinity of these complexes to the active centre of enzymes. It seems fruitful to apply cobalt-59 NMR in this physico-biochemical area.

11. SEVERAL RECENT TOPICS

11.1. Hexanitrocobaltate(III)

The well-known pigment "Aureolin", and characteristic potassium precipitant, sodium hexanitrocobaltate(III) is seemingly the complex of longest history among the numerous cobalt(II) complexes. However, there are some unclarified problems with this complex mainly in aqueous solution and the magnitude of CFSE. Detailed crystal structure analysis and vibrational spectroscopic data confirmed the "hexanitro" or "hexanitrito-N" type coordination, but the different characteristics between the absorption spectra in aqueous solution and photoacoustic or reflectance spectra of the solid state suggests that some different species may exist when in aqueous solution.

From the first cobalt-59 NMR report by Proctor and Yu,[5] it has been suggested that there are different species which show larger chemical shifts from the main signals. These species were further studied by Gasser and Richards[9] and the existence of nitro–nitrito linkage isomers has been suggested. Rose and Bryant studied this complex by cobalt-59 and nitrogen-14 NMR relaxation, and estimated the coupling constant $^1J(^{59}\text{Co}-^{14}\text{N})$[75–77] from both spectra.

Watabe[127] synthesized nitrogen-15 labelled sodium hexanitrocobaltate(III) and recorded the cobalt-59 NMR spectra in aqueous solution buffered with TRIS (pH = 8.3), and found the finely resolved multiplet spectra of cobalt-59 from the spin–spin coupling with ligand nitrogen-15 ($I = 1/2$).

This multiplet was a symmetric sextet, and much different from the septet expected from the coordination of six nitrogen atoms. This means that the cobalt(III) species in the aqueous hexanitrocobaltate(III) solution contains only five nitrogen ligand atoms. He concluded that the existing species in this solution should be $[\text{Co}(\text{NO}_2)_5(\text{OH})]^{3-}$ or $[\text{Co}(\text{NO}_2)_5(\text{OH}_2)]^{2-}$ (pH dependent) with the aid of the electrophoretic characteristics. His conclusion suggests that the absorption maximum at around 380 nm should be the lower-energy part of the doublet of C_{4v} type complexes, which has been assumed to the d–d transition of octahedrally symmetric cobalt(III) complexes. It is also expected that there must be a much larger contribution by the lowest excited state to the chemical shift of cobalt-59 than the second excited state.

Recent solid-state cobalt-59 NMR[122] data might support this conclusion, because the trend of the chemical shift change of hexanitrocobaltate(III) between solution and solid state is opposite to that of the well-established hexaamminecobalt(III) or tris(acetylacetonato(cobalt(II)) complexes.

11.2. NMR Thermometer

The large temperature dependence of the cobalt-59 chemical shift had been already pointed out in the earliest paper by Proctor and Yu.[5] Recent improvement of NMR spectrometers made it possible to determine exactly the change of chemical shift in the order of 0.1 ppm for sharp spectral lines. There are several proposals, of which the most reasonable one is tris(acetylacetonato)cobalt(III) in toluene or potassium hexacyanocobaltate(III) in aqueous solution.

11.3. Solid-State NMR

Recent developments in CP/MAS technique have been well applied to the many samples of half-spin nuclides, such as carbon-13 and silicon-29. The sharp spectra of many quadrupolar nuclides including cobalt-59 seem difficult to observe because of the large anisotropy of chemical shift tensors. Only several well-grown single crystals were chosen for the determination of chemical shift anisotropy.

Several highly-symmetric cobalt complexes were recorded by magic-angle spinning NMR spectroscopy.[122,126] The large chemical shift anisotropies of these complexes showed remarkable field dependence of spectral features as expected. The average chemical shifts are, however, not so different from the liquid samples. It means that the electronic surroundings of the central cobalt-59 nucleus do not change remarkably as a whole.

11.4. Database Construction

As in proton and carbon-13 NMR, the NMR spectroscopic data of cobalt-59 can be utilized as a powerful tool for characterization of various diamagnetic species in solutions such as mother liquors used in synthesis. Intensely coloured specimens usually prevent almost all spectroscopic measurements such as Raman, infrared, or visible-ultraviolet spectroscopy. The "in situ" characterization of the reacting species can be successfully examined by cobalt-59 NMR if accumulation and specification of spectroscopic data have been carried out.

Some trials were reported by Yamasaki[89] by the use of a large-scale computer equipped with a "personal database system" which was based on the compilation of literature data.[64] However, the improvement of the personal computer has made it possible to construct a "personal-size" database easily. The construction of a cobalt-59 NMR database with dBASE-III software was also reported.[128]

12. CONCLUSION

Many useful applications of cobalt-59 NMR are to be expected in the inorganic and organometallic chemistry, as noted by Laszlo[3] in his review. The accumulation of spectroscopic data in a computer-readable form would be necessary for further applications in such a broad research area.

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List of Abbreviations for ligands, solvents and substituents

Am	amyl (pentyl)
Bu	butyl
Bz	benzyl
CHD	1,3-cyclohexadiene
CHT	1,3,5-cycloheptatriene
COD	cyclooctadiene
DMF	dimethylformamide

DMSO	dimethylsulfoxide
Et	ethyl
HIm	imidazole
Hex	hexyl
Me	methyl
MeIm	methylimidazole
OEP	octaethylporphinato(2-)
Oct	octyl
Ph	phenyl
Pr	propyl
Py	pyridyl
TMEDA	tetramethylethylenediamine
TPP	tetraphenylporphinato(2-)
TTA	thenoyltrifluoroacetonato(-)
ThioA	thioacetamide
ThioS	thiosemicarbazide
ThioU	thiourea
abu	aminobutyrato(-)
acac	acetylacetonato(-)
acac-Br	3-bromo-acetylacetonato(-)
acac-NO_2	3-nitro-acetylacetonato(-)
acacen	bis(acetylacetone)ethylenediiminato(2-)
acacpn	bis(acetylacetone)propylenediiminato(2-)
aibu	aminoisobutyrato(-)
ala	alaninato(-)
amben	bis(*o*-aminobenzaldehyde)ethylenediiminato(2-)
atc	acetylcamphorato(-)
bdn	1,3-butanediamine
benacen	bis(benzoylacetone)ethylenediiminato(2-)
bimp	1,3-bis(biacetylmonooximimino)(-)
bipy	2,2′-bipyridine
bn	tetramethylenediamine (1,4-butanediamine)
bzac	benzoylacetonato(-)
c-Hex	cyclohexyl
dbzm	dibenzoylmethanato(-)
dbzm-S	monothio-benzoylmethanato(-)
diars	*o*-phenylenebis(dimethylarsine)
dien	diethylenetriamine
diphos	*o*-phenylenebis(dimethylphosphine)
dmgH	dimethylglyoximato(-)
dpm	dipivaloylmethanato(-)
edta	ethylenediaminetetraacetato(4-)
en	ethylenediamine
fod	heptafluoro-dimethyl-octanedionato(-)
gly	glycinato(-)
hmcar	hydroxymethylenecarvonato(-)
ibn	isobutylenediamine
ileu	isoleucinato(-)
inaa	isonitrosoacetylacetonato(-)
ketox	*o*-hydroxyacetophenone-oximato(-)

leu	leucinato(-)
mal	malonato(2-)
mbn	meso-2,3-butanediamine
morph	morpholino-
mptn	2-methyl-2,4-pentanediamine
nleu	norleucinato(-)
nva	norvalinato(-)
phen	1,10-phenanthroline
pic	picoline
pip	piperidino-
pn	propylenediamine
ppd	phenylpropanedionato(-)
ptn	2,4-pentanediamine
pyrr	pyrrolidino-
sacaen	bis(thioacetylacetone)ethylenediiminato(2-)
salen	bis(salicylidene)ethylenediiminato(2-)
salox	salicylaldoximato(-)
salphen	bis(salicylidene)-*o*-phenylenediiminato(2-)
tacn	triazacyclononane
tame	1,1,1-tris(aminomethyl)methane
tetraen	tetraethylenepentamine
tfac	trifluoroacetylacetonato(-)
tn	trimethylenediamine
tol	toluidine
triarsine	$(CH_3)_2As(CH_3)_3A_s(CH_3)_3As(CH_3)_2As$(??)
trien	triethylenetetramine
trop	tropolonato(-)
val	valinato(-)

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