Diamagnetic Corrections and Pascal's Constants

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Laboratory experiments involving measurement of magnetic susceptibilities (χ, the ability of a substance to be attracted to or repelled by an external magnetic field) have had longstanding success in the undergraduate curriculum. Many experiments suitable for laboratory courses in physical chemistry or inorganic chemistry focus on the determination of the number of unpaired electrons in various transition-metal salts (1–6). These experiments present students with a special set of challenges, one of the most confusing and frustrating of which is the use of tabulated diamagnetic susceptibilities or empirical Pascal's constants that are used to correct for the fundamental or underlying diamagnetism of a paramagnetic compound. Many sources (1, 2, 7–15) contain selected (i.e., incomplete) tabulated data, and often conflicting values are given in different sources owing to the different interpretations of diamagnetic susceptibilities that arose in the early 20th century (8). In this article we present an explanation for the origin of the diamagnetic correction factors, organized tables of constants compiled from other sources (1, 2, 7–17), a link to a new interactive online resource for these tables, a simple method for estimating the correct order of magnitude for the diamagnetic correction for any given compound, a clear explanation of how to use the tabulated constants to calculate the diamagnetic susceptibility, and a worked example for the magnetic susceptibility of copper acetate.

Unlike paramagnetism (attraction of a substance to a magnetic field, a property of compounds having nonzero spin or orbital angular momentum), diamagnetism (repulsion from a magnetic field) is a property of *all* atoms in molecules. Whereas paramagnetism arises from the presence of unpaired electrons in a molecule, all electrons, whether paired or unpaired, cause diamagnetism. It is the conflict between paramagnetism and diamagnetism that defines the overall (measured) magnetic susceptibility, χ_{meas}, which is positive for paramagnetic substances and negative for diamagnetic substances. Paramagnetic contributions to the measured susceptibility, or paramagnetic susceptibility χ_P, are positive and temperature-dependent (for a Curie paramagnet, χ_P is proportional to $1/T$ where T is temperature). Diamagnetic susceptibilities, χ_D, are temperature independent and are negative. The total measured magnetic susceptibility, χ_{meas}, is defined as the sum of these contributions:

$$\chi_{meas} = \chi_P + \chi_D \qquad (1)$$

Thus a compound having unpaired electrons but with an abundance of other paired electrons, such as a metalloprotein (18), may display diamagnetism at room temperature in a bulk measurement.

For room temperature magnetic susceptibility measurements carried out in an undergraduate laboratory, the goal is determination of χ_P using

$$\chi_P = \chi_{meas} - \chi_D \qquad (2)$$

The paramagnetic susceptibility can be related to the number of unpaired electrons in the molecule by eq 3a, a specialized form

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of the more general eq 3 that assumes $g = 2$,

$$\chi_P T = \frac{N_A\, g^2\, \beta^2}{3\, k_B} \left[S(S + 1) \right] \qquad (3)$$

$$\chi_P T = \frac{1}{8}\, n\,(n + 2) \qquad (3a)$$

where T is absolute temperature, N_A is Avogadro's constant, g is the Landé factor or electronic magnetogyric constant, β is the Bohr magneton, k_B is the Boltzmann constant, S is the overall spin state of the molecular substance, and n is the number of unpaired electrons.

Values of χ_D are obtained from literature sources that may list data for whole molecules, fragments of molecules, or individual atoms, ions, or bonds. It is important to pay close attention to the sign of tabulated data, for example, ref 16 lists diamagnetic susceptibilities for organic molecules as $-\chi$; that is, the table contains positive values but they must be treated as negative values for use in eq 2. The same volume, however, lists magnetic susceptibilities for elements and inorganic compounds as χ, so these values should be used as given. For convenience, we compile here tables of diamagnetic susceptibilities from various sources in Tables 1–6 (1, 2, 7–17); where data from two or more sources conflicted, we have generally chosen the more precise value.

Contents of the Tables

In his original publications (19–21), Pascal proposed that the diamagnetism of a molecule could be determined in an additive fashion using values for the diamagnetic susceptibility of every atom (χ_{Di}) and bond (λ_i) in the molecule:

$$\chi_D = \sum_i \chi_{Di} + \sum_i \lambda_i \qquad (4)$$

The values of χ_{Di} and λ_i became known as "Pascal's constants". One source of confusion about Pascal's constants stems from the fact that the values of these constants were often revised during Pascal's lifetime (22, 23), leading to the propagation of several conflicting values cited in different texts. The main reason for revising the original constants was to remove the λ "constitutive corrections" by introducing specialized χ_{Di} values (e.g., χ_{Di} for an O atom in a carbonyl group is often cited as $+1.7 \times 10^{-6}$ emu mol^{-1}). Since many of these revised values can be derived directly from Pascal's original set of constants (e.g., $\chi_D(O) + \lambda(C=O)$ $= +1.7 \times 10^{-6}$ emu mol^{-1}), the values cited in Tables 1 and 2 are kept as close as possible to Pascal's original premise (eq 4). This formulation of Pascal's constants also allows for their greater versatility, at the expense of some insignificant accuracy.

Tables 3–6 contain pre-determined χ_{Di} values for important groups of atoms or ions. Specifically, Table 6 contains χ_{Di} values for cations assuming that they are present in purely *ionic* compounds (note that the atomic χ_{Di} values in Table 1 assume that the atoms are present in purely *covalent* species). Consequently, various values in Table 1 and Table 6 are seldom used (e.g., the values for alkali metals in Table 1 and the value for the
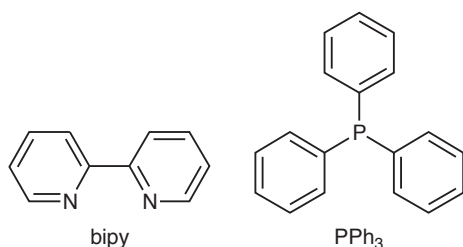
Figure 1. Molecular structures of bipy and PPh₃.

N^{5+} ion in Table 6), but are included for the sake of completeness. Table 3 contains the corresponding χ_{Di} values for anions in completely ionic environments. Tables 4 and 5 contain χ_{Di} values for whole molecules that may be present as ligands or solvents of crystallization. Note that no λ_i values are presented for bonds to metals in coordination compounds. Coordination complexes are assumed to behave as ionic species such that the value of χ_D will be determined by the sum of the ionic contributions of the metal ion(s) from Table 6 and the corresponding values for the ligands from Tables 3 or 4. Precision of the data in Tables 1–6 is an issue worth discussing since the number of significant figures in the data varies drastically from one to three or four. Many of the data are thus imprecise, and, as will be discussed later, the improved precision of some values is not entirely necessary since even a 10% change in χ_D does not have a significant influence in the derived χ_P values for paramagnetic species (~1%) and will not

influence the determination of the number of unpaired electrons in a molecule. When determining χ_D from the values in Tables 1–6, we therefore round our derived values at the decimal.

Using the Tables

Tables 3–6 are the easiest to use; these values may be included in eq 4 as given. Values of χ_{Di} for species not included in Tables 3–6 may be determined from data in Tables 1 and 2 by adding up the values for all constituent atoms as given in Table 1 and for all bonds given in Table 2. For diamagnetic molecules or ligands in routine use, the reader may extend Table 4 or Table 5 by either calculating values as described above or simply obtaining χ_{meas} for the pure substance experimentally. These tables are available at *JCE* ChemInfo: Inorganic, where readers can submit and archive χ_{Di} values for substances of their own interest *(24)*.

As a measure of the efficacy of eq 4, we have measured χ_D at room temperature for two common ligands listed in Table 4, 2,2′-dipyridyl (bipy) and triphenylphosphine (PPh₃), shown in Figure 1, using an Alfa Aesar magnetic susceptibility balance Mark 1. The measured values were χ_D (bipy) = -91×10^{-6} emu mol⁻¹ and χ_D (PPh₃) = -160×10^{-6} emu mol⁻¹ and the tabulated values are χ_D (bipy) = -105×10^{-6} emu mol⁻¹ and χ_D (PPh₃) = -167×10^{-6} emu mol⁻¹, which are in reasonable agreement with experiment (Note: the unit emu is not an SI unit but is the most widely used unit for magnetic susceptibility; 1 emu = 1 cm³).

Table 1. Values of χ_{Di} for Atoms in Covalent Species

Atom	$\chi_{Di}/(1 \times 10^{-6}$ emu mol⁻¹)	Atom	$\chi_{Di}/(1 \times 10^{-6}$ emu mol⁻¹)	Atom	$\chi_{Di}/(1 \times 10^{-6}$ emu mol⁻¹)	Atom	$\chi_{Di}/(1 \times 10^{-6}$ emu mol⁻¹)
Ag	−31.0	C (ring)	−6.24	Li	−4.2	S	−15.0
Al	−13.0	Ca	−15.9	Mg	−10.0	Sb(III)	−74.0
As(III)	−20.9	Cl	− 20.1	N (ring)	−4.61	Se	−23.0
As(V)	−43.0	F	−6.3	N (open chain)	−5.57	Si	−13
B	−7.0	H	−2.93	Na	−9.2	Sn(IV)	−30
Bi	−192.0	Hg(II)	−33.0	O	−4.6	Te	−37.3
Br	− 30.6	I	−44.6	P	−26.3	Tl(I)	−40.0
C	− 6.00	K	−18.5	Pb(II)	−46.0	Zn	−13.5

Table 2. Values of λ_i for Specific Bond Types

Bondᵃ	$\lambda_i/(1 \times 10^{-6}$ emu mol⁻¹)	Bond	$\lambda_i/(1 \times 10^{-6}$ emu mol⁻¹)	Bond	$\lambda_i/(1 \times 10^{-6}$ emu mol⁻¹)	Bond	$\lambda_i/(1 \times 10^{-6}$ emu mol⁻¹)
C=C	+5.5	Cl–CR₂CR₂–Cl	+4.3	Ar–Br	−3.5	Imidazole	+8.0
C≡C	+0.8	R₂CCl₂	+1.44	Ar–Cl	−2.5	Isoxazole	+1.0
C=C–C=C	+10.6	RCHCl₂	+6.43	Ar–I	−3.5	Morpholine	+5.5
Ar–C≡C–Arᵇ	+3.85	C–Br	+4.1	Ar–COOH	−1.5	Piperazine	+7.0
CH₂=CH–CH₂–(allyl)	+4.5	Br–CR₂CR₂–Br	+6.24	Ar–C(=O)NH₂	−1.5	Piperidine	+3.0
C=O	+6.3	C–I	+4.1	R₂C=N–N=CR₂	+10.2	Pyrazine	+9.0
COOH	−5.0	Ar–OH	−1	RC≡C–C(=O)R	+0.8	Pyridine	+0.5
COOR	−5.0	Ar–NR₂	+1	Benzene	−1.4ᶜ	Pyrimidine	+6.5
C(=O)NH₂	−3.5	Ar–C(=O)R	−1.5	Cyclobutane	+7.2	α- or γ-Pyrone	−1.4
N=N	+1.85	Ar–COOR	−1.5	Cyclohexadiene	+10.56	Pyrrole	−3.5
C=N–	+8.15	Ar–C=C	−1.00	Cyclohexane	+3.0	Pyrrolidine	+0.0
–C≡N	+0.8	Ar–C≡C	−1.5	Cyclohexene	+6.9	Tetrahydrofuran	+0.0
–N≡C	+0.0	Ar–OR	−1	Cyclopentane	+0.0	Thiazole	−3.0
N=O	+1.7	Ar–CHO	−1.5	Cyclopropane	+7.2	Thiophene	−7.0
–NO₂	−2.0	Ar–Ar	−0.5	Dioxane	+5.5	Triazine	−1.4
C–Cl	+3.1	Ar–NO₂	−0.5	Furan	−2.5		

ᵃOrdinary C–H and C–C single bonds are assumed to have a λ value of 0.0 emu mol⁻¹. ᵇThe symbol Ar represents an aryl ring. ᶜSome sources list the λ value for a benzene ring as −18.00 to which three times λ(C=C) must then be added. To minimize the calculations involved, this convention was not followed such that λ values given for aromatic rings are assumed to automatically take into account the corresponding double bonds in the ring.

Table 3. Values of χ_{Di} for Anions

Anion	χ_{Di}/(1 × 10⁻⁶ emu mol⁻¹)	Anion	χ_{Di}/(1 × 10⁻⁶ emu mol⁻¹)	Anion	χ_{Di}/(1 × 10⁻⁶ emu mol⁻¹)	Anion	χ_{Di}/(1 × 10⁻⁶ emu mol⁻¹)
AsO_3^{3-}	−51	$C_5H_5^-$	−65	NCO^-	−23	$S_2O_3^{2-}$	−46
AsO_4^{3-}	−60	$C_6H_5COO^-$	−71	NCS^-	−31.0	$S_2O_8^{2-}$	−78
BF_4^-	−37	CO_3^{2-}	−28.0	O^{2-}	−12.0ª	HSO_4^-	−35.0
BO_3^{3-}	−35	$C_2O_4^{2-}$	−34	OAc^-	−31.5	Se^{2-}	−48ᵇ
Br^-	−34.6	F^-	−9.1	OH^-	−12.0	SeO_3^{2-}	−44
BrO_3^-	−40	$HCOO^-$	−17	PO_3^{3-}	−42	SeO_4^{2-}	−51
Cl^-	−23.4	I^-	−50.6	$PtCl_6^{2-}$	−148	SiO_3^{2-}	−36
ClO_3^-	−30.2	IO_3^-	−51	S^{2-}	−30	Te^{2-}	−70
ClO_4^-	−32.0	IO_4^-	−51.9	SO_3^{2-}	−38	TeO_3^{2-}	−63
CN^-	−13.0	NO_2^-	−10.0	SO_4^{2-}	−40.1	TeO_4^{2-}	−55
		NO_3^-	−18.9				

ªThe value of χ_{Di} for O^{2-} is reported as −6.0 in some sources. ᵇThis value is uncertain.

Table 4. Values of χ_{Di} for Common Ligands

Ligand	χ_{Di}/(1 × 10⁻⁶ emu mol⁻¹)	Ligand	χ_{Di}/(1 × 10⁻⁶ emu mol⁻¹)	Ligand	χ_{Di}/(1 × 10⁻⁶ emu mol⁻¹)	Ligand	χ_{Di}/(1 × 10⁻⁶ emu mol⁻¹)
$Acac^-$	−52	Ethylene	−15	NH_3	−18	Pyrazine	−50
Bipy	−105	Glycinate	−37	Phen	−128	Pyridine	−49
CO	−10	H_2O	−13	o-PBMA	−194	$Salen^{2-}$	−182
$C_5H_5^-$	−65	Hyrdazine	−20	Phthalocyanine	−442	Urea	−34
En	−46.5	Malonate	−45	PPh_3	−167		

NOTE: Abbreviations: acac = acetylacetonate, bipy = 2,2'-dipyridyl, en = ethylenediamine, phen = phenanthroline, PBMA = phenylenebisdimethylarsine, salen = ethylenebis(salicylaminate)

Table 5. Values of χ_{Di} for Common Solvents of Crystallization

Solvent	χ_{Di}/(1 × 10⁻⁶ emu mol⁻¹)	Solvent	χ_{Di}/(1 × 10⁻⁶ emu mol⁻¹)	Solvent	χ_{Di}/(1 × 10⁻⁶ emu mol⁻¹)	Solvent	χ_{Di}/(1 × 10⁻⁶ emu mol⁻¹)
CCl_4	−66.8	CH_3CN	−27.8	$CH_3C(=O)OC(=O)CH_3$	−52.8	Cyclohexane	−68
$CHCl_3$	−58.9	$1,2\text{-}C_2H_4Cl_2$	−59.6	$CH_3CH_2CH_2CN$	−50.4	Hexane	−74.1
CH_2Cl_2	−46.6	CH_3COOH	−31.8	$CH_3C(=O)OCH_2CH_3$	−54.1	Triethylamine	−83.3
CH_3Cl	−32.0	CH_3CH_2OH	−33.7	$CH_3CH_2CH_2CH_2OH$	−56.4	Benzonitrile	−65.2
CH_3NO_2	−21.0	$HOCH_2CH_2OH$	−38.9	$CH_3CH_2OCH_2CH_3$	−55.5	Toluene	−65.6
CH_3OH	−21.4	CH_3CH_2SH	−44.9	Pentane	−61.5	Isooctane	−99.1
CCl_3COOH	−73.0	$CH_3C(=O)CH_3$	−33.8	o-Dichlorobenzene	−84.4	Naphthalene	−91.6
CF_3COOH	−43.3			Benzene	−54.8		

Values of χ_D for bipy and PPh_3 may also be determined from Pascal's constants (Tables 1 and 2) as follows:

$$\chi_D(\text{bipy}) = 10\,\chi_D(C_{\text{ring}}) + 2\,\chi_D(N_{\text{ring}}) + 8\,\chi_D(H)$$
$$+ 2\,\lambda(\text{pyridine}) + \lambda(\text{Ar–Ar})$$
$$= [10(-6.24) + 2(-4.61) + 8(-2.93)$$
$$+ 2(0.5) + (-0.5)] \times 10^{-6}\,\text{emu mol}^{-1}$$
$$= -95 \times 10^{-6}\,\text{emu mol}^{-1}$$

$$\chi_D(PPh_3) = \chi_D(P) + 18\,\chi_D(C_{\text{ring}})$$
$$+ 15\,\chi_D(H) + 3\,\lambda(\text{benzene})$$
$$= [-26.3 + 18(-6.24) + 15(-2.93)$$
$$+ 3(-1.4)] \times 10^{-6}\,\text{emu mol}^{-1}$$
$$= -187 \times 10^{-6}\,\text{emu mol}^{-1}$$

As a check, the computed value of χ_D should be close to the value estimated by the following equation

$$\chi_D \approx -\frac{MW}{2} 10^{-6}\,\text{emu mol}^{-1} \qquad (5)$$

where MW is the (unitless) molecular weight of the substance (9). In fact, for situations where great accuracy is not needed (such as for a room temperature measurement in an undergraduate lab), use of eq 5 can be sufficient for determining χ_D. For comparison, the χ_D values for bipy and PPh_3 estimated from eq 5 are −78 × 10⁻⁶ emu mol⁻¹ and −131 × 10⁻⁶ emu mol⁻¹.

For magnetic susceptibility measurements of metalloenzymes, in which χ_{meas} is dominated by χ_D, an accurate method for determining χ_D is necessary. This is typically achieved by measuring the susceptibility of the protein without the metal included or on a homolog of the protein having a diamagnetic metal center in place of the paramagnetic metal (18). This technique emphasizes the fact that the most accurate χ_D values can only be obtained by measurement.

Table 6. Values of χ_{Di} for Cations

Cation	$\chi_{Di}/(1 \times 10^{-6}$ emu mol$^{-1})$	Cation	$\chi_{Di}/(1 \times 10^{-6}$ emu mol$^{-1})$	Cation	$\chi_{Di}/(1 \times 10^{-6}$ emu mol$^{-1})$
Ag^+	−28	Ir^{4+}	−29	Rh^{4+}	−18
Ag^{2+}	−24[a]	Ir^{5+}	−20	Ru^{3+}	−23
Al^{3+}	−2	K^+	−14.9	Ru^{4+}	−18
As^{3+}	−9[a]	La^{3+}	−20	S^{4+}	−3
As^{5+}	−6	Li^+	−1.0	S^{6+}	−1
Au^+	−40[a]	Lu^{3+}	−17	Sb^{3+}	−17[a]
Au^{3+}	−32	Mg^{2+}	−5.0	Sb^{5+}	−14
B^{3+}	−0.2	Mn^{2+}	−14	Sc^{3+}	−6
Ba^{2+}	−26.5	Mn^{3+}	−10	Se^{4+}	−8
Be^{2+}	−0.4	Mn^{4+}	−8	Se^{6+}	−5
Bi^{3+}	−25[a]	Mn^{6+}	−4	Si^{4+}	−1
Bi^{5+}	−23	Mn^{7+}	−3	Sm^{2+}	−23
Br^{5+}	−6	Mo^{2+}	−31	Sm^{3+}	−20
C^{4+}	−0.1	Mo^{3+}	−23	Sn^{2+}	−20
Ca^{2+}	−10.4	Mo^{4+}	−17	Sn^{4+}	−16
Cd^{2+}	−24	Mo^{5+}	−12	Sr^{2+}	−19.0
Ce^{3+}	−20	Mo^{6+}	−7	Ta^{5+}	−14
Ce^{4+}	−17	N^{5+}	−0.1	Tb^{3+}	−19
Cl^{5+}	−2	NH_4^+	−13.3	Tb^{4+}	−17
Co^{2+}	−12	$N(CH_3)_4^+$	−52	Te^{4+}	−14
Co^{3+}	−10	$N(C_2H_5)_4^+$	−101	Te^{6+}	−12
Cr^{2+}	−15	Na^+	−6.8	Th^{4+}	−23
Cr^{3+}	−11	Nb^{5+}	−9	Ti^{3+}	−9
Cr^{4+}	−8	Nd^{3+}	−20	Ti^{4+}	−5
Cr^{5+}	−5	Ni^{2+}	−12	Tl^+	−35.7
Cr^{6+}	−3	Os^{2+}	−44	Tl^{3+}	−31
Cs^+	−35.0	Os^{3+}	−36	Tm^{3+}	−18
Cu^+	−12	Os^{4+}	−29	U^{3+}	−46
Cu^{2+}	−11	Os^{6+}	−18	U^{4+}	−35
Dy^{3+}	−19	Os^{8+}	−11	U^{5+}	−26
Er^{3+}	−18	P^{3+}	−4	U^{6+}	−19
Eu^{2+}	−22	P^{5+}	−1	V^{2+}	−15
Eu^{3+}	−20	Pb^{2+}	−32.0	V^{3+}	−10
Fe^{2+}	−13	Pb^{4+}	−26	V^{4+}	−7
Fe^{3+}	−10	Pd^{2+}	−25	V^{5+}	−4
Ga^{3+}	−8	Pd^{4+}	−18	VO^{2+}	−12.5
Ge^{4+}	−7	Pm^{3+}	−27	W^{2+}	−41
Gd^{3+}	−20	Pr^{3+}	−20	W^{3+}	−36
H^+	0	Pr^{4+}	−18	W^{4+}	−23
Hf^{4+}	−16	Pt^{2+}	−40	W^{5+}	−19
Hg^{2+}	−40.0	Pt^{3+}	−33	W^{6+}	−13
Ho^{3+}	−19	Pt^{4+}	−28	Y^{3+}	−12
I^{5+}	−12	Rb^+	−22.5	Yb^{2+}	−20
I^{7+}	−10	Re^{3+}	−36	Yb^{3+}	−18
In^{3+}	−19	Re^{4+}	−28	Zn^{2+}	−15.0
Ir^+	−50	Re^{6+}	−16	Zr^{4+}	−10
Ir^{2+}	−42	Re^{7+}	−12		
Ir^{3+}	−35	Rh^{3+}	− 22		

[a]This value is uncertain.

A Practical Example: Copper(II) Acetate Hydrate

A possible experiment for an undergraduate inorganic chemistry lab or physical chemistry lab is to determine the magnetic susceptibility of dimeric copper(II) acetate hydrate, $Cu_2(OAc)_4(H_2O)_2$, and relate this value to the number of unpaired electrons per copper atom. Here, we will use Tables 1–6 to determine the diamagnetic correction factor (χ_D) for $Cu_2(OAc)_4(H_2O)_2$. First, we estimate the value of χ_D from eq 5 [the molecular weight of $Cu_2(OAc)_4(H_2O)_2$ is 399.3].

$$\chi_D\left[Cu_2(OAc)_4(H_2O)_2\right]$$
$$= -\frac{399.3}{2} \times 10^{-6}\,emu\,mol^{-1}$$
$$= -200 \times 10^{-6}\,emu\,mol^{-1}$$

A more accurate value of χ_D can be calculated from the following values using Table 3, 4, and 6:

$$\chi_D\left[Cu_2(OAc)_4(H_2O)_2\right]$$
$$= 2\,\chi_D\left(Cu^{2+}\right) + 4\,\chi_D\left(OAc^-\right) + 2\,\chi_D\left(H_2O\right)$$
$$= \left[2(-11) + 4(-31.5)\right.$$
$$\left. + 2(-13)\right] \times 10^{-6}\,emu\,mol^{-1}$$
$$= -174 \times 10^{-6}\,emu\,mol^{-1}$$

Using an Alfa Aesar magnetic susceptibility balance Mark 1, we determined χ_{meas} for a sample of $Cu_2(OAc)_4(H_2O)_2$ to be $+1.30 \times 10^{-3}$ emu mol^{-1} at a temperature of 296.5 K. We now determine χ_P using the χ_D value we determined from Tables 3, 4, and 6:

$$\chi_P = \chi_{meas} - \chi_D$$
$$= \left[1300 - (-174)\right] \times 10^{-6}\,emu\,mol^{-1}$$
$$= 1470 \times 10^{-6}\,emu\,mol^{-1}$$

To relate this value to the number of unpaired electrons in the molecule, we may determine the value of $\chi_P T$ or, alternatively, μ_{eff} (effective magnetic moment), which is an older convention but still widely used:

$$\chi_P T = \left(1470 \times 10^{-6}\,emu\,mol^{-1}\right) 296.5\,K$$
$$= 0.436\,emu\,K\,mol^{-1}$$

$$\mu_{eff} = \sqrt{\frac{3\,k_B}{N_A\,\beta^2}\left(\chi_P T\right)}$$
$$= \sqrt{8\left(1470 \times 10^{-6}\,emu\,mol^{-1}\right) 296.5\,K}$$
$$= 1.87\,\mu_B$$

Note that the value of μ_{eff} is given in units of μ_B or Bohr magnetons. Students should see that $Cu_2(OAc)_4(H_2O)_2$ has somewhere between one and two unpaired electrons, since the unpaired electrons on each copper atom are antiferromagnetically coupled.

If the approximated value of χ_D, -200×10^{-6} emu mol^{-1}, is used in the above calculations, values of $\chi_P T = 0.445$ emu K mol^{-1} and $\mu_{eff} = 1.89\,\mu_B$ are obtained, which differ from the more accurate values by only 1–2% and therefore do not affect the conclusions that may be drawn by the students.

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