

## Pascal's Constants and Constitutive Corrections

**How do you calculate the diamagnetic correction of ligands and ions not listed on the table of diamagnetic corrections for the common ions and ligands?**

**The diamagnetic correction of any ligand or ion can be determined by applying what are called the constitutive corrections.**

Atom/Ion/Species	$\chi_{\text{dia}}$	Atom/Ion/Species	$\chi_{\text{dia}}$	Bond	$\chi_{\text{dia}}$
H	-2.93	F	-6.3	C (in ring)	-0.24
C	-6.00	Cl	-20.1	C (shared by two rings)	-3.07
N (open chain)	-5.57	Br	-30.6	C=C	+5.5
N (monoamide)	-4.61	I	-44.6	C $\equiv$ C	+0.8
N (diamide, imide)	-1.54	S	-15.0	C=N	+8.15
O (alcohol, ether)	-2.11	P	-26.3	C $\equiv$ N	+0.8
O (aldehyde, ketone)	-4.61	As(III)	-20.9	N=N	+1.8
O <sub>2</sub> (carboxylate)	+1.73	As(V)	-43.0	N=O	+1.7
		Sb(III)	-74.0		
		Se	-23.0		

**NOTE: These values need to be multiplied by  $10^{-6}$  to obtain the diamagnetic correction**

**Example:**

**The diamagnetic correction of pyridine ( $\text{C}_5\text{H}_5\text{N}$ )**

$$\begin{aligned}
 5 \times \text{C} &= -30.00 \times 10^{-6} \\
 5 \times \text{H} &= -14.65 \times 10^{-6} \\
 1 \times \text{N}(\text{ring}) &= -4.61 \times 10^{-6} \\
 5 \times \text{C}(\text{ring}) &= -1.20 \times 10^{-6}
 \end{aligned}$$

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$$\text{-50.46} \times 10^{-6} \text{ cgs unit}$$

**Please note that there are corrections for not only the atom, but for the type of bond. In the above example 5 carbon atoms are used, but a further correction is applied since the 5 carbon atoms are in a ring.**