

## Electronic Supplementary Information

The A and B expressions in Van Vleck equation are afforded as follows  
for the fitting of the susceptibility data.

$$\chi = \frac{Ng^2\beta^2}{3kT} \left[ \frac{A}{B} \right]$$

$$\begin{aligned} A = & 1224 \exp\left(\frac{32J_1 + 20J_2}{kT}\right) + 1386 \exp\left(\frac{16J_1 + 20J_2}{kT}\right) + 546 \exp\left(\frac{2J_1 + 20J_2}{kT}\right) + 414 \exp\left(\frac{-10J_1 + 20J_2}{kT}\right) \\ & + 294 \exp\left(\frac{-20J_1 + 20J_2}{kT}\right) + 30 \exp\left(\frac{-34J_1 + 20J_2}{kT}\right) + 6 \exp\left(\frac{-38J_1 + 20J_2}{kT}\right) + 840 \exp\left(\frac{24J_1 + 20J_2}{kT}\right) \\ & + 546 \exp\left(\frac{10J_1 + 20J_2}{kT}\right) + 510 \exp\left(\frac{-2J_1 + 20J_2}{kT}\right) + 180 \exp\left(\frac{12J_1 + 20J_2}{kT}\right) + 84 \exp\left(\frac{-28J_1 + 20J_2}{kT}\right) \\ & + 30 \exp\left(\frac{-26J_1 + 20J_2}{kT}\right) + 6 \exp\left(\frac{8J_1 + 20J_2}{kT}\right) + 330 \exp\left(\frac{4J_1 + 20J_2}{kT}\right) + 180 \exp\left(\frac{-6J_1 + 20J_2}{kT}\right) \\ & + 84 \exp\left(\frac{-14J_1 + 20J_2}{kT}\right) + 330 \exp\left(\frac{-34J_1 + 20J_2}{kT}\right) + 180 \exp\left(\frac{20J_2}{kT}\right) + 840 \exp\left(\frac{24J_1 + 12J_2}{kT}\right) \\ & + 546 \exp\left(\frac{10J_1 + 12J_2}{kT}\right) + 415 \exp\left(\frac{-2J_1 + 12J_2}{kT}\right) + 294 \exp\left(\frac{-12J_1 + 12J_2}{kT}\right) + 84 \exp\left(\frac{-20J_1 + 12J_2}{kT}\right) \\ & + 30 \exp\left(\frac{-26J_1 + 12J_2}{kT}\right) + 6 \exp\left(\frac{-30J_1 + 12J_2}{kT}\right) + 546 \exp\left(\frac{18J_1 + 12J_2}{kT}\right) + 510 \exp\left(\frac{6J_1 + 12J_2}{kT}\right) \\ & + 180 \exp\left(\frac{-4J_1 + 12J_2}{kT}\right) + 30 \exp\left(\frac{-18J_1 + 12J_2}{kT}\right) + 6 \exp\left(\frac{-22J_1 + 12J_2}{kT}\right) + 331 \exp\left(\frac{12J_1 + 12J_2}{kT}\right) \\ & + 180 \exp\left(\frac{2J_1 + 12J_2}{kT}\right) + 84 \exp\left(\frac{-6J_1 + 12J_2}{kT}\right) + 6 \exp\left(\frac{-16J_1 + 12J_2}{kT}\right) + 30 \exp\left(\frac{-8J_1 + 12J_2}{kT}\right) \\ & + 84 \exp\left(\frac{12J_2}{kT}\right) + 546 \exp\left(\frac{16J_1 + 6J_2}{kT}\right) + 415 \exp\left(\frac{4J_1 + 6J_2}{kT}\right) + 300 \exp\left(\frac{-6J_1 + 6J_2}{kT}\right) \\ & + 84 \exp\left(\frac{-14J_1 + 6J_2}{kT}\right) + 30 \exp\left(\frac{-20J_1 + 6J_2}{kT}\right) + 360 \exp\left(\frac{-12J_1 + 6J_2}{kT}\right) + 210 \exp\left(\frac{-2J_1 + 6J_2}{kT}\right) \\ & + 6 \exp\left(\frac{-16J_1 + 6J_2}{kT}\right) + 180 \exp\left(\frac{8J_1 + 6J_2}{kT}\right) + 114 \exp\left(\frac{6J_2}{kT}\right) + 6 \exp\left(\frac{-10J_1 + 6J_2}{kT}\right) \\ & + 330 \exp\left(\frac{8J_1 + 2J_2}{kT}\right) + 324 \exp\left(\frac{2J_1 - 2J_2}{kT}\right) + 84 \exp\left(\frac{-10J_1 + 2J_2}{kT}\right) + 180 \exp\left(\frac{6J_1 + 2J_2}{kT}\right) \\ & + 300 \exp\left(\frac{-8J_1 + 2J_2}{kT}\right) + 84 \exp\left(\frac{4J_1 + 2J_2}{kT}\right) + 6 \exp\left(\frac{-6J_1 + 2J_2}{kT}\right) + 6 \exp\left(\frac{2J_1 + 2J_2}{kT}\right) + 6 \exp\left(\frac{2J_2}{kT}\right) + 325 \end{aligned}$$

$$\begin{aligned}
B = & 17 \exp\left(\frac{32J_1 + 20J_2}{kT}\right) + 28 \exp\left(\frac{16J_1 + 20J_2}{kT}\right) + 13 \exp\left(\frac{2J_1 + 20J_2}{kT}\right) + 18 \exp\left(\frac{-10J_1 + 20J_2}{kT}\right) \\
& + 21 \exp\left(\frac{-20J_1 + 20J_2}{kT}\right) + 7 \exp\left(\frac{-28J_1 + 20J_2}{kT}\right) + 5 \exp\left(\frac{-34J_1 + 20J_2}{kT}\right) + 3 \exp\left(\frac{-38J_1 + 20J_2}{kT}\right) \\
& + \exp\left(\frac{-40J_1 + 20J_2}{kT}\right) + 15 \exp\left(\frac{24J_1 + 20J_2}{kT}\right) \\
& + 13 \exp\left(\frac{10J_1 + 20J_2}{kT}\right) + 20 \exp\left(\frac{-2J_1 + 20J_2}{kT}\right) + 9 \exp\left(\frac{-12J_1 + 20J_2}{kT}\right) + 5 \exp\left(\frac{-26J_1 + 20J_2}{kT}\right) \\
& + 3 \exp\left(\frac{-30J_1 + 20J_2}{kT}\right) + 11 \exp\left(\frac{4J_1 + 20J_2}{kT}\right) + 9 \exp\left(\frac{-6J_1 + 20J_2}{kT}\right) \\
& + 7 \exp\left(\frac{-14J_1 + 20J_2}{kT}\right) + 11 \exp\left(\frac{8J_1 + 20J_2}{kT}\right) + 9 \exp\left(\frac{20J_2}{kT}\right) + 15 \exp\left(\frac{24J_1 + 12J_2}{kT}\right) \\
& + 13 \exp\left(\frac{10J_1 + 12J_2}{kT}\right) + 18 \exp\left(\frac{-2J_1 + 12J_2}{kT}\right) + 21 \exp\left(\frac{-12J_1 + 12J_2}{kT}\right) + 7 \exp\left(\frac{-20J_1 + 12J_2}{kT}\right) \\
& + 5 \exp\left(\frac{-26J_1 + 12J_2}{kT}\right) + 3 \exp\left(\frac{-30J_1 + 12J_2}{kT}\right) + 13 \exp\left(\frac{18J_1 + 12J_2}{kT}\right) + 20 \exp\left(\frac{6J_1 + 12J_2}{kT}\right) \\
& + 9 \exp\left(\frac{-4J_1 + 12J_2}{kT}\right) + 5 \exp\left(\frac{-18J_1 + 12J_2}{kT}\right) + 3 \exp\left(\frac{-22J_1 + 12J_2}{kT}\right) + \exp\left(\frac{-24J_1 + 12J_2}{kT}\right) \\
& + 11 \exp\left(\frac{12J_1 + 12J_2}{kT}\right) + 9 \exp\left(\frac{-2J_1 + 12J_2}{kT}\right) + 7 \exp\left(\frac{-6J_1 + 12J_2}{kT}\right) + 3 \exp\left(\frac{-16J_1 + 12J_2}{kT}\right) + 5 \exp\left(\frac{-8J_1 + 12J_2}{kT}\right) \\
& + 7 \exp\left(\frac{12J_2}{kT}\right) + 13 \exp\left(\frac{16J_1 + 6J_2}{kT}\right) + 18 \exp\left(\frac{4J_1 + 6J_2}{kT}\right) + 24 \exp\left(\frac{-6J_1 + 6J_2}{kT}\right) \\
& + 7 \exp\left(\frac{-14J_1 + 6J_2}{kT}\right) + 5 \exp\left(\frac{-20J_1 + 6J_2}{kT}\right) + 17 \exp\left(\frac{-12J_1 + 6J_2}{kT}\right) + 14 \exp\left(\frac{-2J_1 + 6J_2}{kT}\right) \\
& + 3 \exp\left(\frac{-16J_1 + 6J_2}{kT}\right) + 9 \exp\left(\frac{8J_1 + 6J_2}{kT}\right) + 12 \exp\left(\frac{6J_2}{kT}\right) + 3 \exp\left(\frac{-10J_1 + 6J_2}{kT}\right) \\
& + 11 \exp\left(\frac{8J_1 + 2J_2}{kT}\right) + 26 \exp\left(\frac{2J_1 - 2J_2}{kT}\right) + 7 \exp\left(\frac{-10J_1 + 2J_2}{kT}\right) + 9 \exp\left(\frac{6J_1 + 2J_2}{kT}\right) \\
& + 5 \exp\left(\frac{-8J_1 + 2J_2}{kT}\right) + 7 \exp\left(\frac{4J_1 + 2J_2}{kT}\right) + 3 \exp\left(\frac{-6J_1 + 2J_2}{kT}\right) + 3 \exp\left(\frac{2J_1 + 2J_2}{kT}\right) + \exp\left(\frac{-4J_1 + 2J_2}{kT}\right) + 3 \exp\left(\frac{2J_2}{kT}\right) + 25
\end{aligned}$$