
\[ J = \frac{[E(SBS) - E(T)]}{[1 + S_{ab}^2]} \]

where \( S_{ab} \) is the overlap between the SOMO orbitals of each fragment. For through-space interactions \( S_{ab} \approx 0 \) and \( J = [E(SBS) - E(T)] \). For through-bond interaction, sometimes \( S_{ab} \) is close to 1 and then \( J = [E(SBS) - E(T)]/2 \). Note that the relative order of \( J_1, J_2 \) and \( J_3 \) and their assignation to the experimental values is not affected by the expressions employed, given the much smaller value of \( J_1 \) in any case.