Previous studies (R. Caballol, O, Castell, F. Illas, I. de P. R. Moreira, J. P. Malrieu, *J. Phys. Chem. A* 1997, *101*, 7860) have shown that $J = [E(SBS)-E(T)]/[1+S_{ab}^2]$, 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.