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A theoretical study of the effects of polar substitution on the activation barriers for internal rotation around the C-N bond in p-substituted nitrosobenzenes: comparison of DFT and MP2 calculations

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Abstract: The activation barriers for internal rotation around the C-N bond in p-substituted nitrosobenzenes were calculated using the density functional theory (DFT) and second-order Møller-Plesset (MP2) methods with the 6-31+g(d) basis set. The polarisable continuum model (PCM) was used to model the solvent effect. An explicit water molecule was also introduced to form a hydrogen bond with the nitrosogroup and its effect on the barrier was studied by DFT. The barriers were well-correlated with Hammett sigma^{+} rather than