

Negligible Ability of Oxygen and Peroxide Ion Activation by Al(III) Ion Is Essential for Al(III)-Induced Neurodegeneration

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The electron densities of the atoms in Fe(II)- or Al(III)-tyrosine hydroxylase (THO) containing oxygen and pterin were calculated by the DFT (Density-functional theory) method. The results obtained are consistent with our previous proposal that oxygen activation in THO proceeds through the formation of an intermediate derived from Fe(II), oxygen, and pterin. Electron donation from substrate to the oxygen molecule is important to cleave the O-O bond, and to give the hydroxylated product. Based on these results, it was concluded that hydroxylation of the aromatic ring does not proceed in the Al(III)-containing THO, and a relationship exists between Al(III) ion and neurodegeneration.