Probing the hydride transfer process in the lumiflavine-1- methylnicotinamide model system using group softness

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The hydride transfer process between the isoalloxazine moiety of flavins and the nicotinamide moiety of NAD(P)H has been explored by using density functional theory based reactivity index in the 1-methylnicotinamide-lumiflavine model system. Based on crystallographic data available, we have found that the group softness index helps to locate and orientate reactive regions in these interacting molecules while the electrophilicity index successfully describes the reactivity pattern of this system.