Theoretical study of the local reactivity of electrophiles of the type MPR 3 + (M=Cu, Ag, Au ;R=-H, -Me, -Ph)

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Reactivity prediction in the series of MPR 3 + fragments (M=Au, Ag, Cu; R=-H, -Me, -Ph) has been achieved at the ab initio (HF and MP2) and density functional theory (B3LYP and PBE) levels. We have used global and local descriptors based on conceptual DFT such as hardness, Fukui function and electrophilicity index. For all methods and fragments, we have found an equal trend in reactivity using both the global and local electrophilicity index: QR-AuPR 3 + >CuPR 3 +?AgPR 3 +>NR-AuPR 3 +. It is also found that the electrophilicity power decreases as the volume of R increases.