Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

σ-Aromatic Cyclic M_3^+ (M = Cu, Ag, Au) Clusters and their Complexation with Dimethyl imidazol-2-ylidene, Pyridine, Isoxazole, Furan, Noble Gas and Carbon Monoxide

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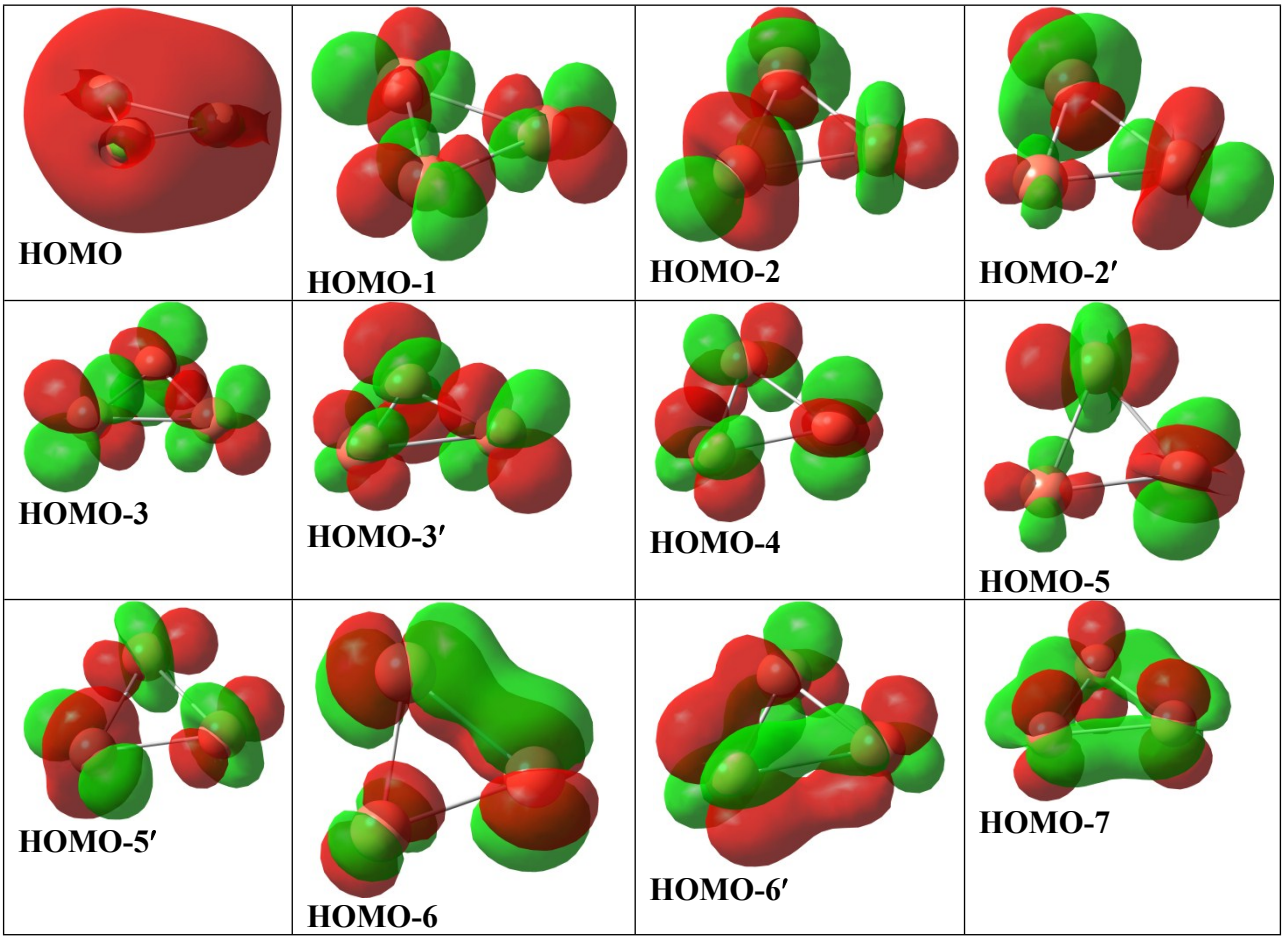
Supporting Information



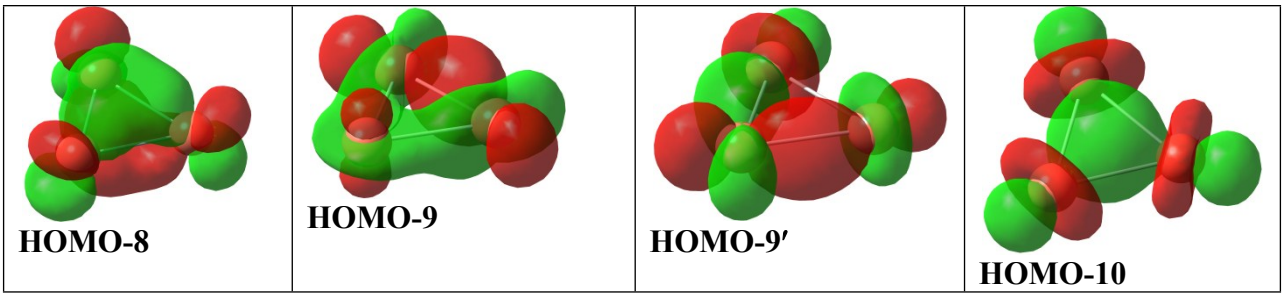


Fig. 1-SI Occupied molecular orbitals of M_3^+.

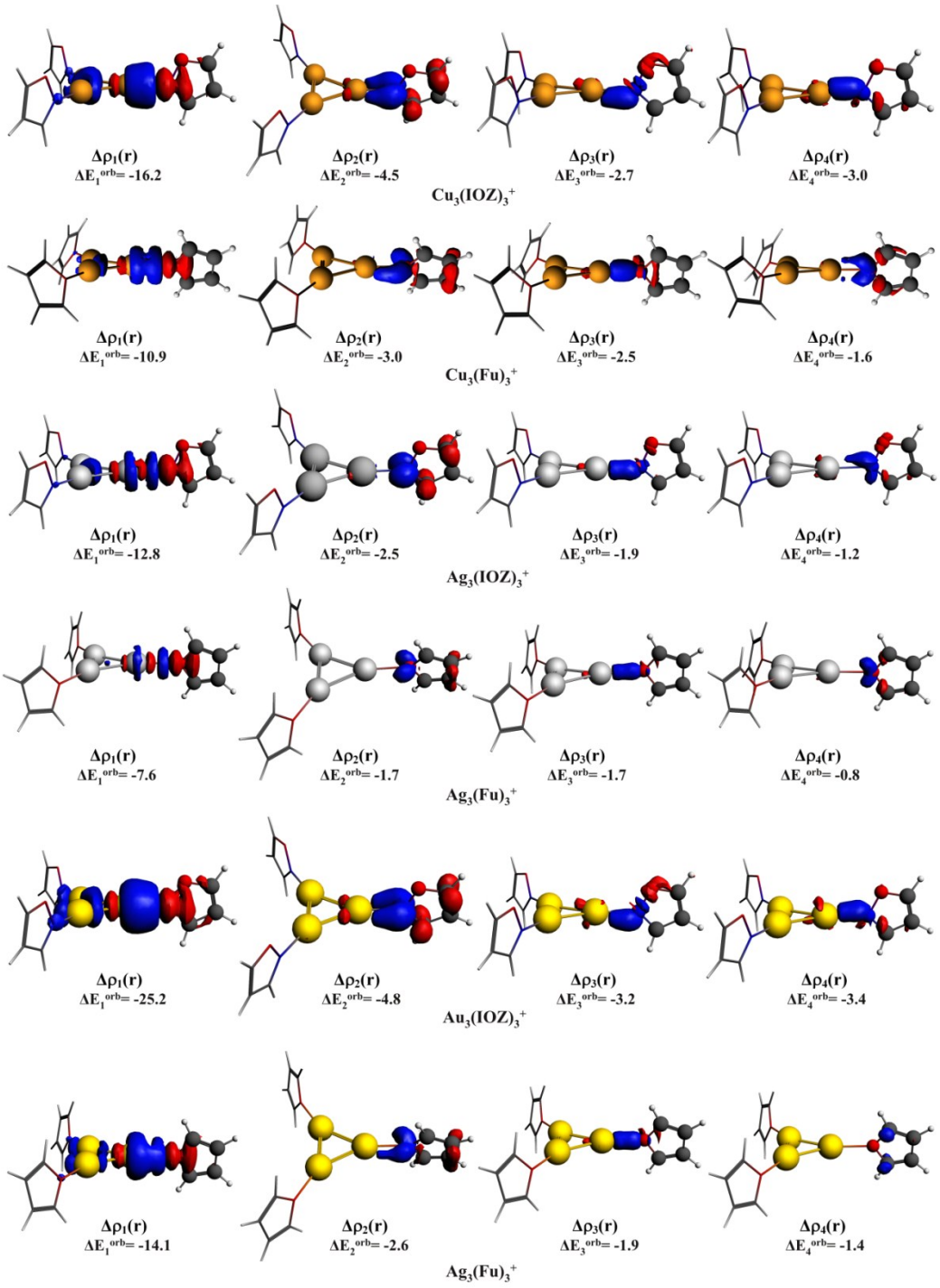


Fig. 2-SI The plots of deformation density ($\Delta\rho(r)$) for $M_3(IOZ)_3^+$ and $M_3(Fu)_3^+$ complexes at the PBE-D3/TZ2P//M06-2X/def2-TZVP level.

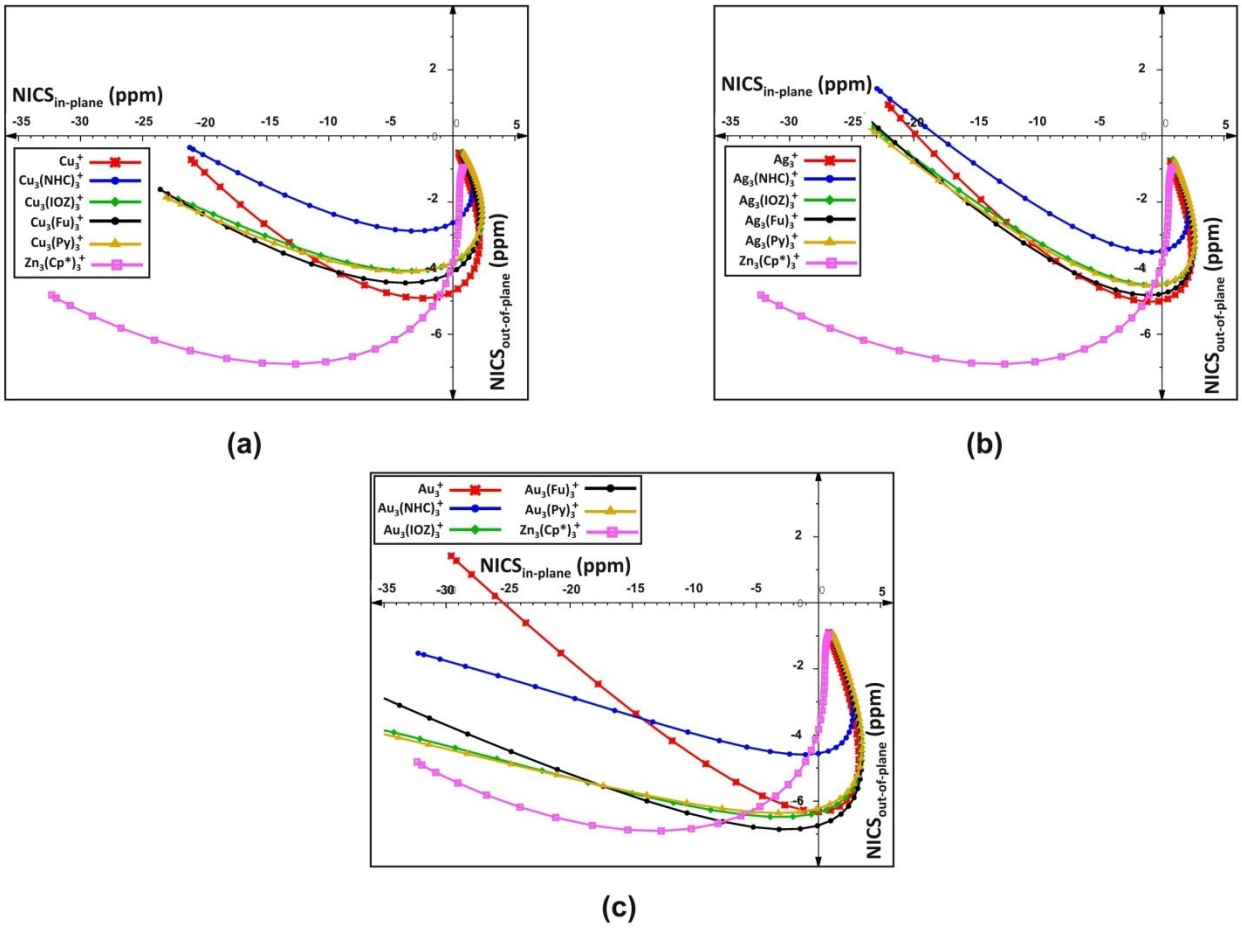


Fig. 3-SI FiPC-NICS plots for the $M_3L_3^+$ complexes at the M06-2X/def2-TZVP level.

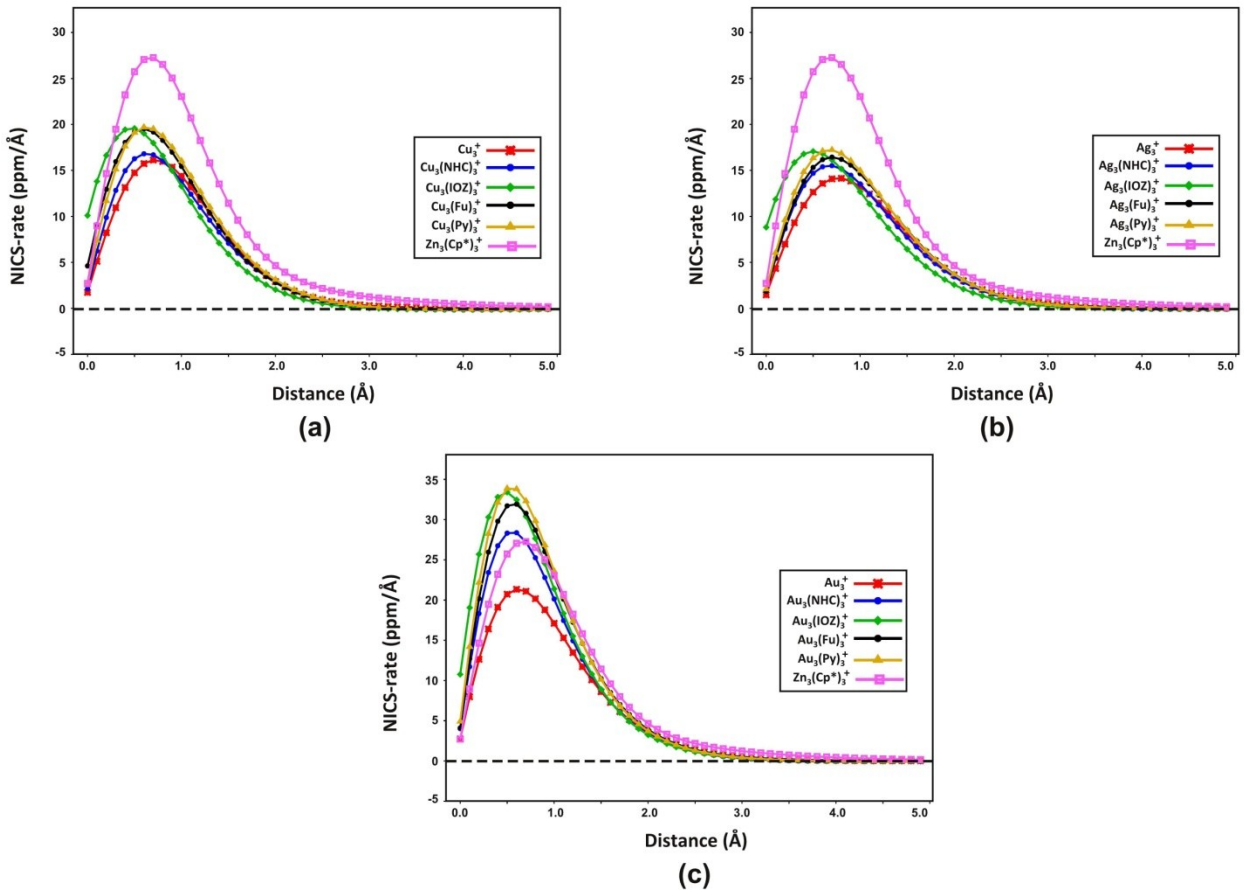


Fig. 4-SI NICS-rate plots for the $M_3L_3^+$ complexes at the M06-2X/def2-TZVP level.

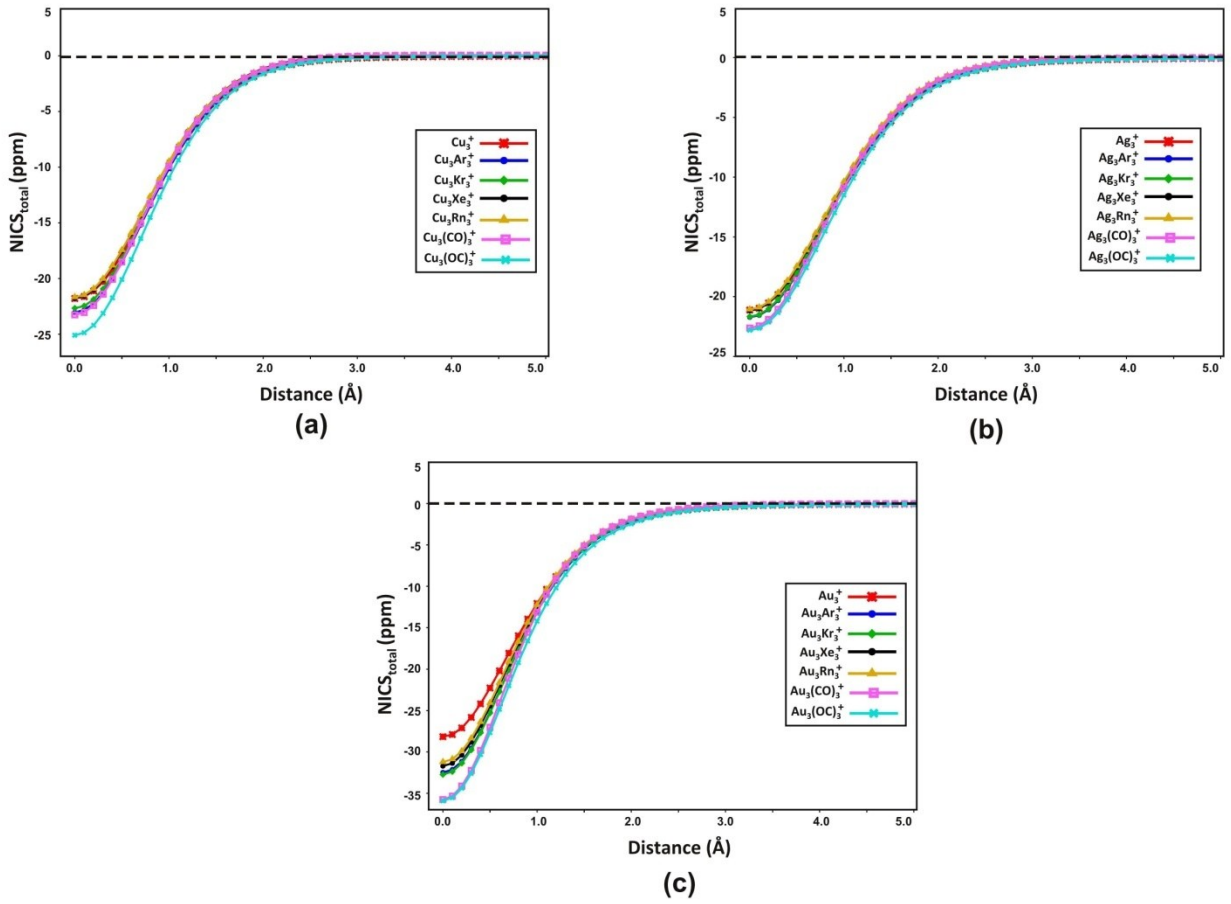


Fig. 5-SI $NICS_{total}$-scan plots for the $M_3Ng_3^+$, $M_3(CO)_3^+$ and $M_3(OC)_3^+$complexes at the M06-2X/def2-TZVP level.

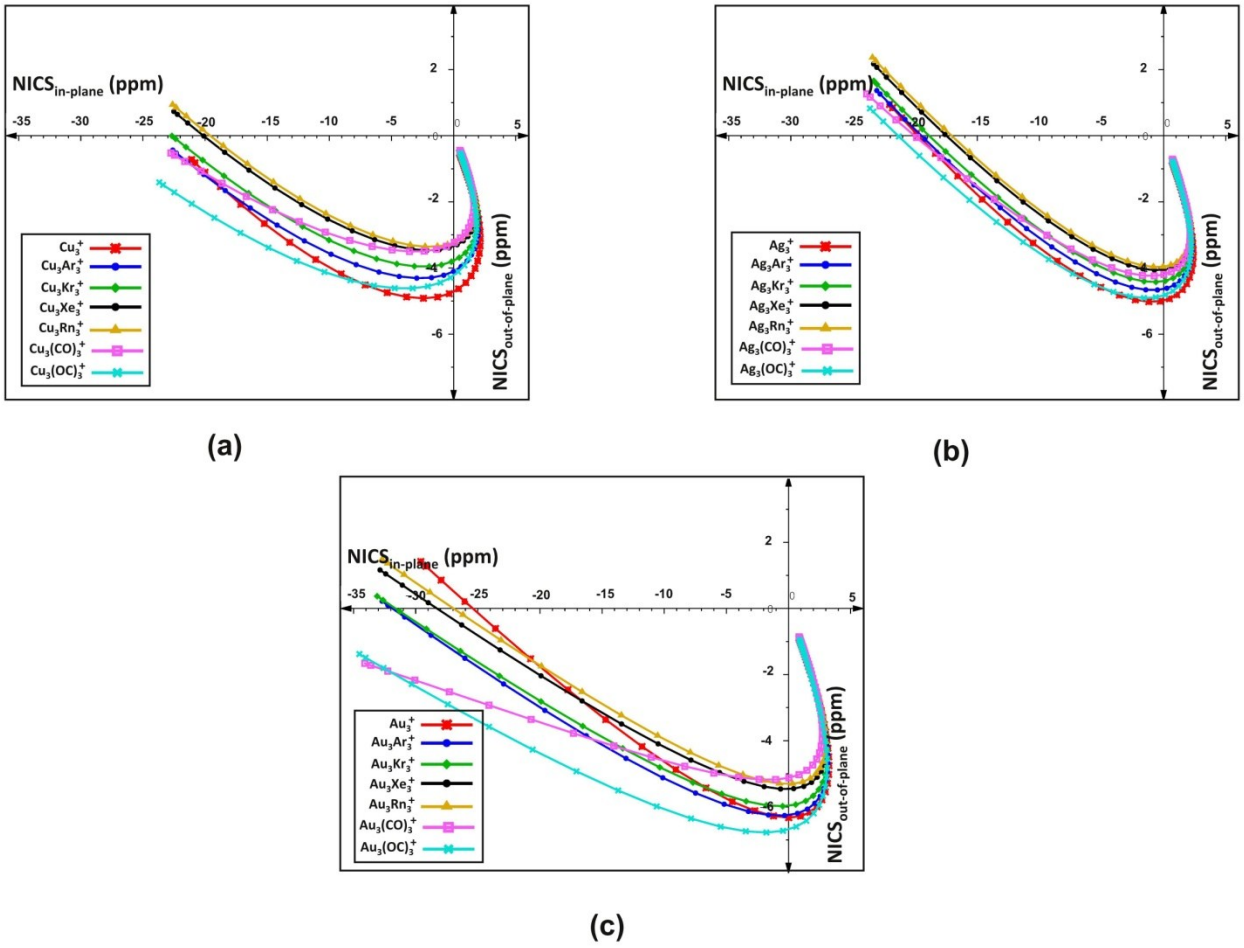


Fig. 6-SI FiPC-NICS plots for the $M_3Ng_3^+$, $M_3(CO)_3^+$ and $M_3(OC)_3^+$complexes at the M06-2X/def2-TZVP level.

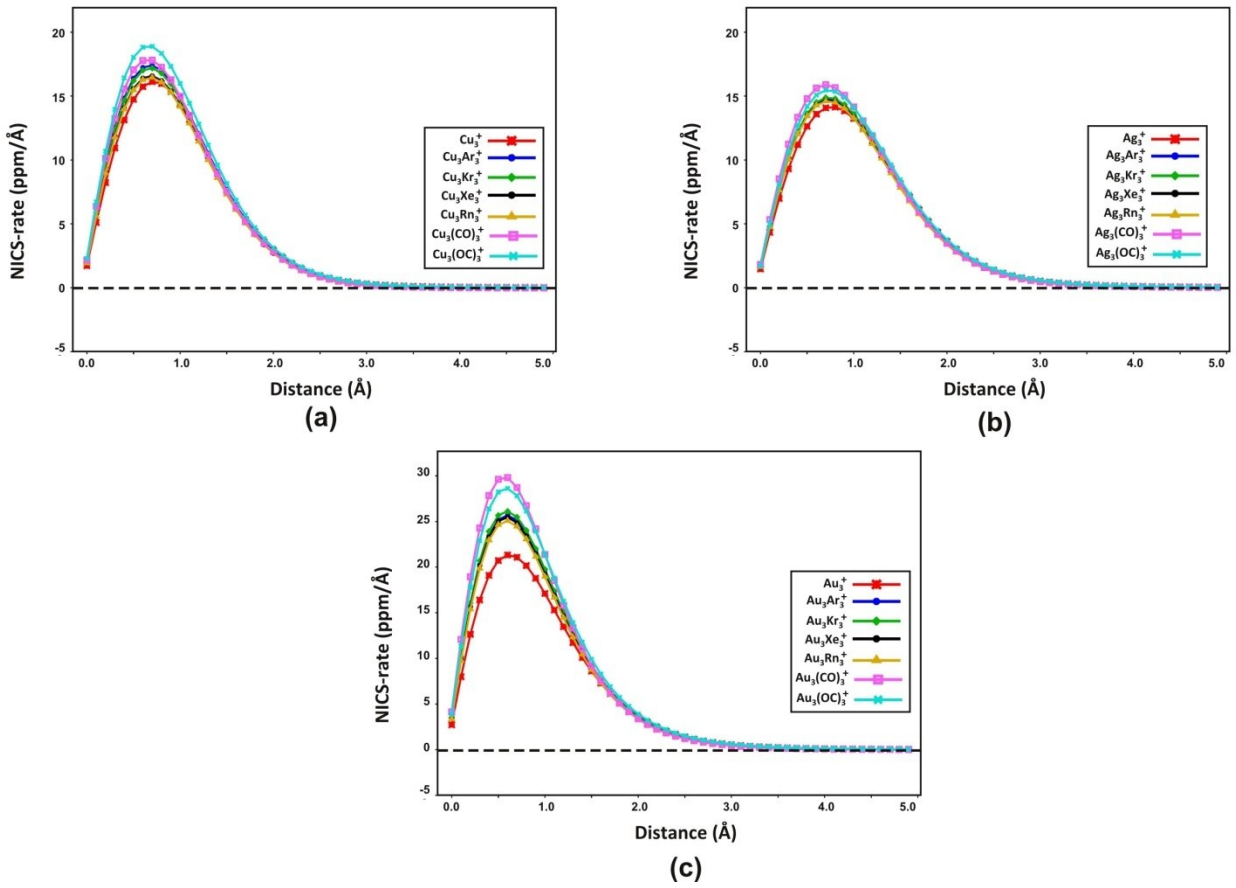


Fig. 7-SI NICS-rate plots for the $M_3Ng_3^+$, $M_3(CO)_3^+$ and $M_3(OC)_3^+$ at the M06-2X/def2-TZVP level.

$Cu_3Ng_3^+$ and $Ag_3Ng_3^+$ systems are close in $NICS_{total}(0)$ and $NICS_{total}(1)$ values to the corresponding bare units whereas $Au_3Ng_3^+$ demonstrates increased $NICS_{total}$ values (see Fig. 5-SI). The in-plane components of the NICS are the major contributors towards the total aromaticity in all these complexes (see Fig. 6-SI). NICS-rate plot shows that the size of the hump increases in $M_3Ng_3^+$ compare to bare moieties (see Fig. 7-SI).

In general, $M_3(OC)_3^+$ molecules show more $NICS_{total}(0)$ values than that of the $M_3(CO)_3^+$, though the difference is small (see Fig. 5-SI). The in-plane components of the NICS increases noticeably in case of $M_3(OC)_3^+$ (see Fig. 6-SI). NICS-rate plot shows increment in the hump size both in $M_3(CO)_3^+$ and $M_3(OC)_3^+$ in comparison to the M_3^+ molecules (see Fig. 7-SI).