Liste des abréviations

ADF	Amsterdam Density Functional
DFT	Density Functional Theory
GGA	Generalized Gradient Approximation
LSDA	Local Spin Density Approximation
HOMO	Highest Occupied Molecular Orbital
LUMO	Lowest Unoccupied Molecular Orbital
υ	Élongation
ς	déformation
IR	Infra-Rouge
GGA	approximation du gradient généralisé L ligand
LDA	Local Density Approximation
L	Ligand