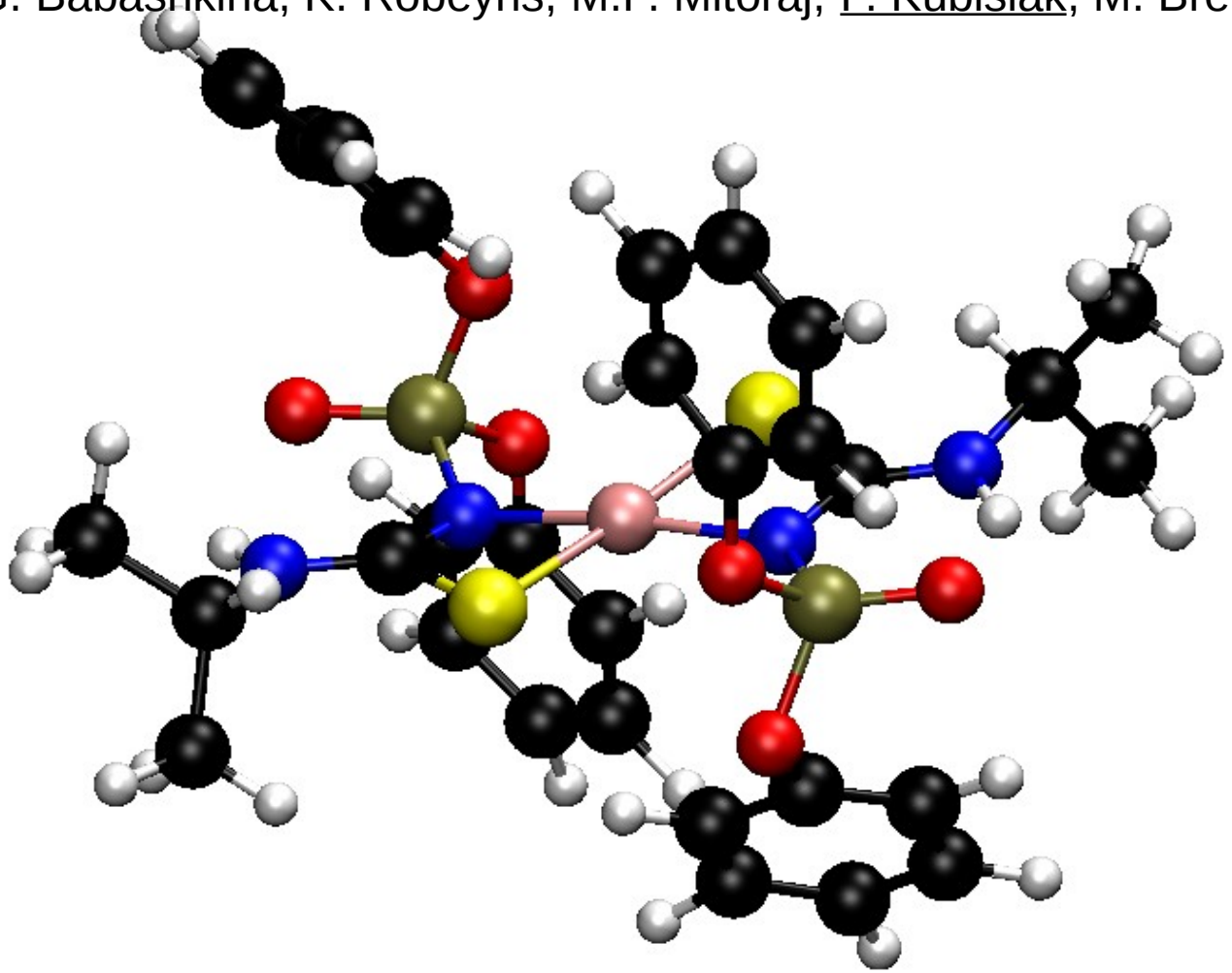
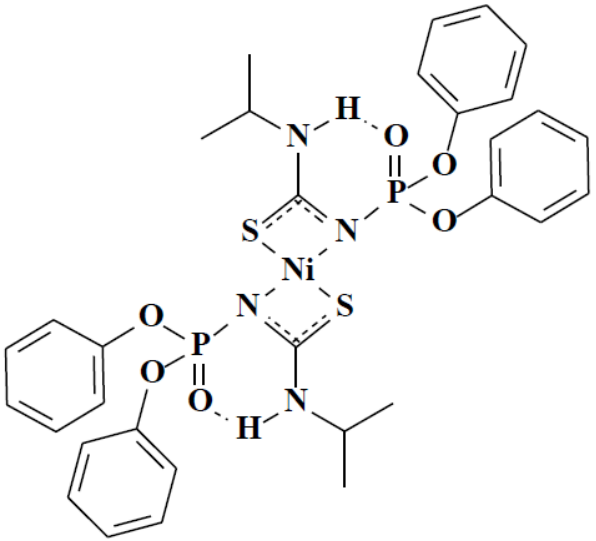
Experimental and theoretical investigations of the Ni^{II} complex with *N*-phosphorylated thiourea *i*PrNHC(S)NHP(O)$(OPh)_2$

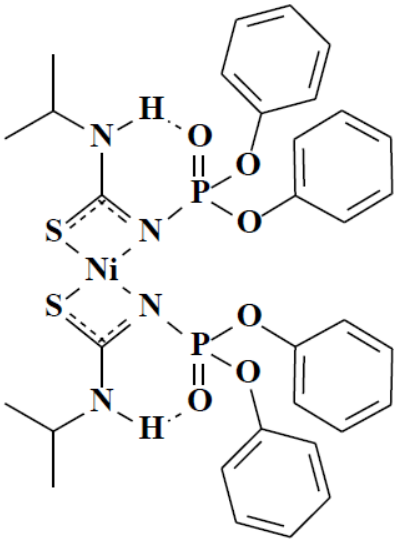
D.A. Safin, M.G. Babashkina, K. Robeyns, M.P. Mitoraj, P. Kubisiak, M. Brela and Y. Garcia



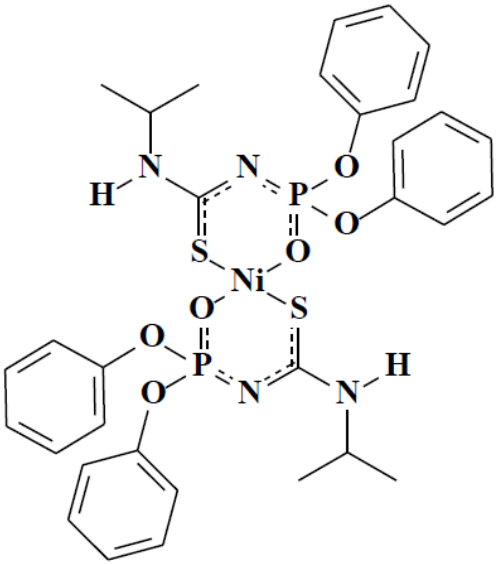
Possible conformations of [NiL_2]



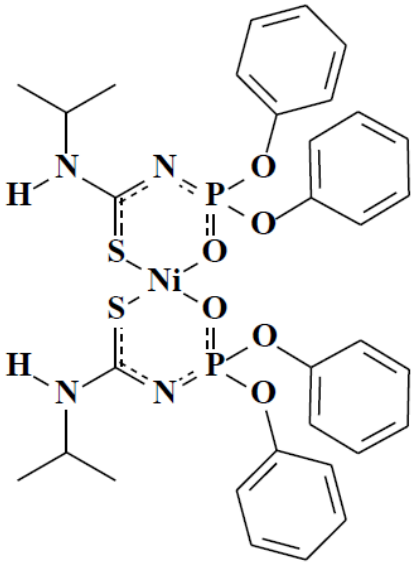
trans-[Ni(L-1,3-*N*,*S*)$_2$]
0.0 kcal/mol and 0.0 kcal/mol



cis-[Ni(L-1,3-*N*,*S*)$_2$]
13.3 kcal/mol and 11.4 kcal/mol



trans-[Ni(L-1,5-*O*,*S*)$_2$]
9.6 kcal/mol and 26.0 kcal/mol



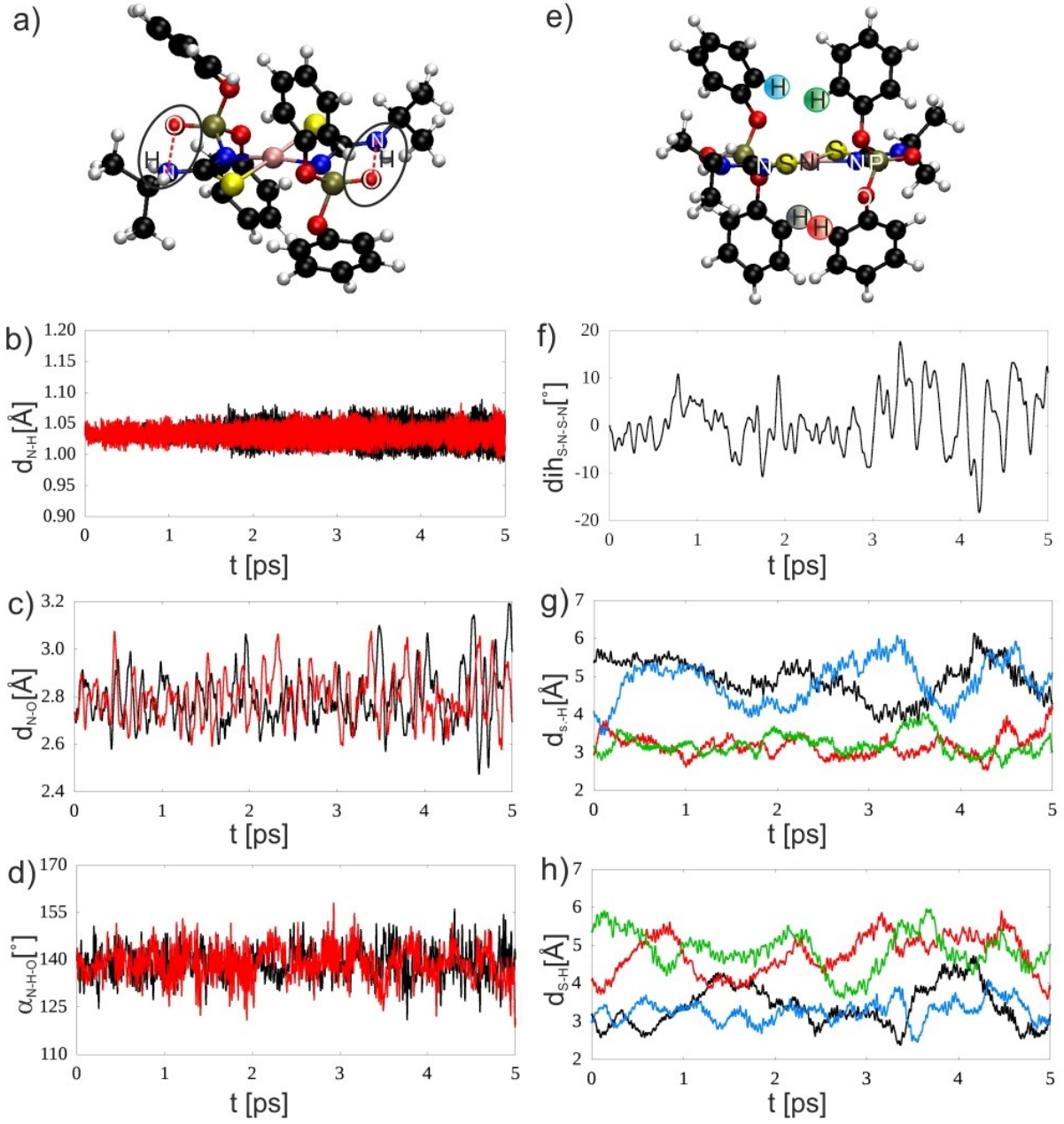
cis-[Ni(L-1,5-*O*,*S*)$_2$]
13.3 kcal/mol and 23.1 kcal/mol

Gaussian 09 package

B3LYP/6-311G**

B97D/6-311G**

Ab initio molecular dynamics



CP2K 2.4 package

DFT based Born-Oppenheimer molecular dynamics simulations

Changes of the selected parameters for the *trans*-1,3-*N,S*-isomer of [NiL_2]

a-d: major characteristics of two hydrogen bonds N–H···O=P (black and red lines)

f: deviations of the dihedral angle S-N-S-N

g-h: changes in the distances between each sulfur atom and four *o*-Ph hydrogen atoms (coded in red, blue, green and black colors)