Supporting Information

DFT/TDDFT study on spectroscopic properties of zinc(II), nickel(II), and palladium(II) metal complexes with thiourea derivative

XIN WANG, JIEQIONG LI, LI WANG*, WENPENG WU*

Institute of Environmental and Analytical Sciences, College of Chemistry and Chemical Engineering, Henan University, Kaifeng 475004, Henan, P.R. China

Table SI Mean unsigned error (MUE) for three different functionals.

Fucntionals	MUE[a]	MUE[b]
B3LYP	0.0389	3.43
B3PW91	0.0269	3.36
M06	0.0286	2.71

[a]based on bondlengths

[b]based on bond angles and dihedral angles

*Corresponding authors.

E-mail: chemwangl@henu.edu.cn(LI WANG), wenpengwu@126.com(WENPENG WU).

Table SII Molecular orbital compositions in the ground state for $Zn(C_{10}H_{12}N_3OS)_2$ (**1**) at M06/6-31+G(d)-LANL2DZ level in dimethylformamide.

MO	Energy	Contribution											Assignment
	(eV)	Py(A)	Py(B)	Mor(A)	Mor(B)	S(1)	S(2)	C(1)	C(3)	N(2)	N(4)	Zn	
L+2	-0.93	37	37	0	0	0	0	0	0	0	0	0	π^*[Py(A)+Py(B)]
L+1	-1.23	14	14	0	0	0	0	0	0	0	0	0	π^*[Py(A)+Py(B)]
L	-1.39	12	12	0	0	0	0	0	0	0	0	0	π^*[Py(A)+Py(B)]
H	-6.37	0	0	0	0	0	0	0	0	13	13	0	p[N(2)+N(4)]
H-1	-6.37	0	0	0	0	0	10	0	0	13	14	0	p[S(2)+N(2)+N(4)]
H-2	-6.78	0	0	0	0	31	31	0	0	0	0	0	p[S(1)+S(2)]
H-3	-6.80	0	0	0	0	29	29	0	0	0	0	0	p[S(1)+S(2)]

Table SIII Molecular orbital compositions in the ground state for $Ni(C_{10}H_{12}N_3OS)_2$ (**2**) at M06/6-31+G(d)-LANL2DZ level in dimethylformamide.

MO	Energy	Contribution											Assignment
	(eV)	Py(A)	Py(B)	Mor(A)	Mor(B)	S(1)	S(2)	C(1)	C(2)	N(2)	N(4)	Ni	
L+2	-1.28	14	14	0	0	0	0	0	0	0	0	0	π^*[Py(A)+Py(B)]
L+1	-1.33	22	22	0	0	0	0	0	0	0	0	0	π^*[Py(A)+Py(B)]
L	-2.10	0	0	0	0	15	15	0	0	0	0	46	p[S(1)+S(2)]+d(Ni)
H	-6.23	0	0	0	0	11	11	0	0	11	11	13	p[S(1)+S(2)+N(2)+N(4)]+d(Ni)
H-1	-6.31	0	0	0	0	17	17	0	0	11	11	0	p[S(1)+S(2)+N(2)+N(4)]
H-2	-6.53	0	0	13	13	13	13	0	0	0	0	12	p[S(1)+S(2)+Mor(A)+Mor(B)]+d(Ni)
H-3	-6.64	0	0	0	0	23	23	0	0	0	0	12	p[S(1)+S(2)]+d(Ni)

Table SIV Molecular orbital compositions in the ground state for $Pd(C_{10}H_{12}N_3OS)_2$ (**3**) at M06/6-31+G(d)-LANL2DZ level in dimethylformamide.

MO	Energy	Contribution											Assignment
	(eV)	Py(A)	Py(B)	Mor(A)	Mor(B)	S(1)	S(2)	C(1)	C(2)	N(2)	N(4)	Pd	
L+2	-1.25	14	14	0	0	0	0	0	0	0	0	0	π^*[Py(A)+Py(B)]
L+1	-1.31	13	13	0	0	0	0	0	0	0	0	0	π^*[Py(A)+Py(B)]
L	-2.31	0	0	0	0	17	17	0	0	0	0	39	p[S(1)+S(2)]+d(Pd)
H	-6.15	0	0	0	0	17	17	0	0	0	0	17	p[S(1)+S(2)]+d(Pd)
H-1	-6.34	0	0	0	0	14	14	0	0	12	12	0	p[S(1)+S(2)+N(2)+N(4)]
H-2	-6.56	0	0	12	12	17	17	0	0	0	0	14	p[S(1)+S(2)+Mor(A)+Mor(B)]+d(Pd)
H-3	-6.64	0	0	0	0	15	15	0	0	0	0	0	p[S(1)+S(2)]

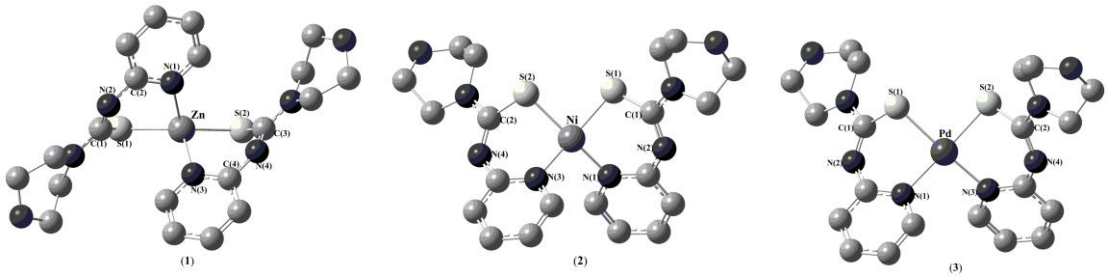

Fig. S1 The optimized ground-state geometrical structures for complexes Zn($C_{10}H_{12}N_3OS)_2$ (**1**), Ni($C_{10}H_{12}N_3OS)_2$ (**2**), and Pd($C_{10}H_{12}N_3OS)_2$ (**3**). The hydrogen atoms are omitted for clarity.