Synthesis, Structure, Thermal Decomposition and Computational Calculation of Heterodinuclear Ni^{II} – Zn^{II} Complexes

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Supporting Information

Table S1. The occupancy values of the atom orbitals obtained from the NBO program.

Complex	Atom	Orbital	Occupied Value
1	N1	p_x	1.31077
		p_y	1.42878
		p_z	1.39082
	N2	p_x	1.31049
		p_y	1.42884
		p_z	1.39073
	N3	p_x	1.39990
		p_y	1.15865
		p_z	1.52475
	N4	p_x	1.57103
		p_y	1.0089
		p_z	1.27452
	N6	p_x	1.44875
		p_y	1.15043
		p_z	1.28560
	N7	p_x	1.28066
		p_y	1.24600
		p_z	1.56585
	Ni	d_{xy}	1.96806
		d_{zx}	1.60339
		d_{yz}	1.14051
		d_{x2-y2}	1.96452
		d_{z2}	1.98120
	Zn	d_{xy}	1.99629
		d_{zx}	1.99780
		d_{yz}	1.99658
		d_{x2-y2}	1.99617
		d_{z2}	1.99570
2	N1	p_x	1.31385
		p_y	1.42805
		p_z	1.38702
	N2	p_x	1.31478
		p_y	1.42792
		p_z	1.38622
	N3	p_x	1.55649
		p_y	1.34542
		p_z	1.18901
	N4	p_x	1.66754
		p_y	1.21593
		p_z	1.18070
	Ni	d_{xy}	1.96904

	d_{zx}	1.71704
	d_{yz}	1.02560
	d_{x2-y2}	1.96293
	d_{z2}	1.98263
Zn	d_{xy}	1.99646
	d_{zx}	1.99783
	d_{yz}	1.99666
	d_{x2-y2}	1.99610
	d_{z2}	1.99556

Table S2. Second-order perturbation analysis results of the atom orbitals obtained from the NBO program.

Complex	Unit of Molecule	Orbital Type (%)
1	Unit 1: $C_{17}H_{16}N_2O_2$ (Schiff base ligand)	TL: 97.2960 TNL:2.4618 TRNL:0.2422
	Unit 2: $C_3H_4N_2$ (pyrazole 1)	TL: 97.3740 TNL:2.4433 TRNL:0.1827
	Unit 3: $C_3H_4N_2$ (pyrazole 2)	TL: 97.1824 TNL:2.6394 TRNL:0.1782
	Unit 4: Ni	TL: 95.1759 TNL:4.7959 TRNL:0.0282
	Unit 5: Zn	TL: 97.0752 TNL:2.9074 TRNL:0.1750
2	Unit 1: $C_{17}H_{16}N_2O_2$ (Schiff base ligand)	TL: 97.4073 TNL:2.3350 TRNL:0.2578
	Unit 2: C_7H_9N (lutidine 1)	TL: 97.5590 TNL:2.2634 TRNL:0.1763
	Unit 3: C_7H_9N (lutidine 2)	TL: 97.5021 TNL:2.3097 TRNL:0.1879
	Unit 4: Ni	TL: 95.2333 TNL:4.7383 TRNL:0.0283
	Unit 5: Zn	TL: 97.0564 TNL:2.9255 TRNL:0.0181

TL: Total Lewis type orbitals, TNL: Total non-Lewis type orbitals, TRNL: Total Rydberg non-Lewis type orbitals

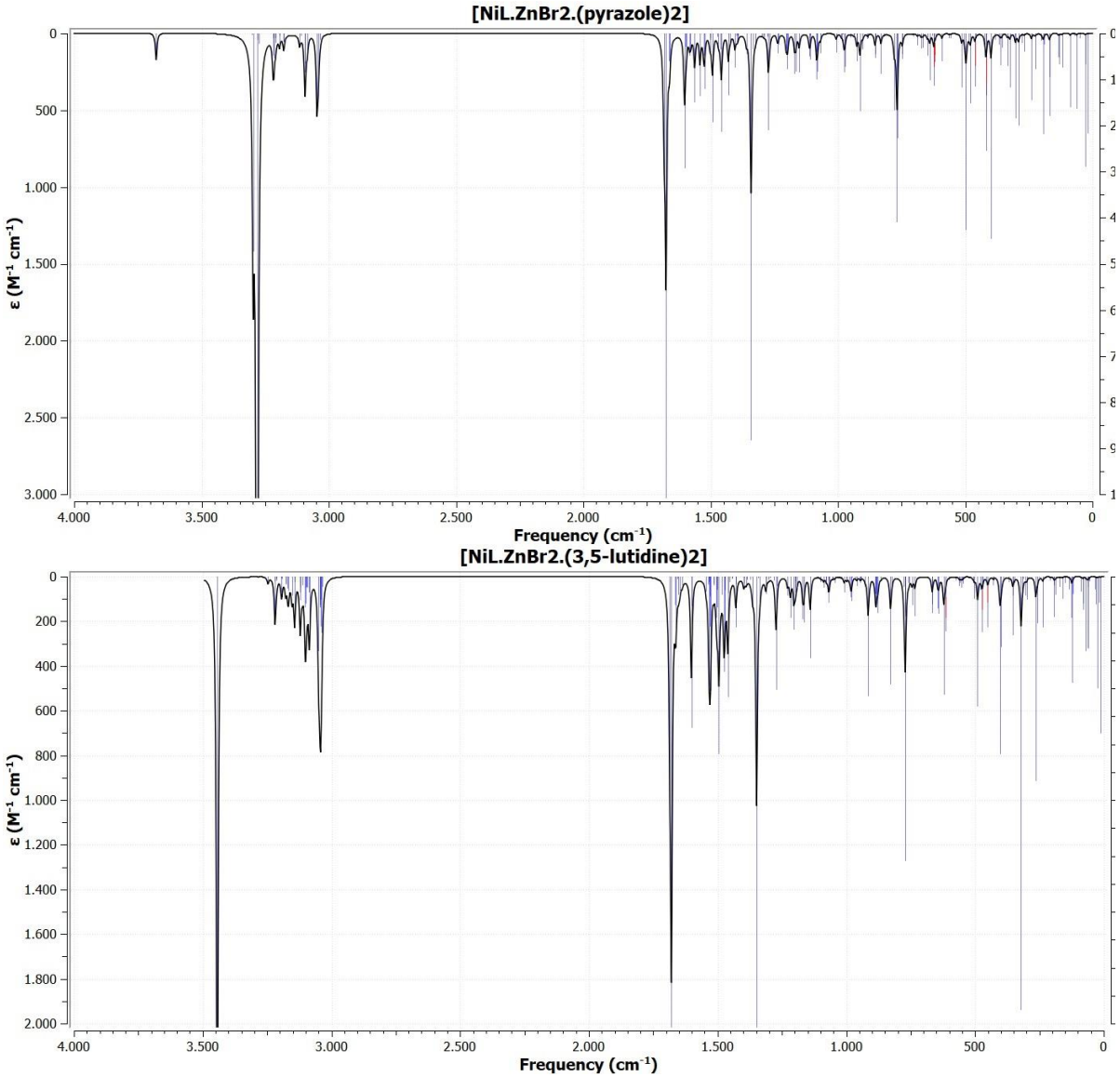

Figure S1. Calculated vibrational wave number (cm^{-1}) assignments of [NiL·$ZnBr_2$·$(pyrazole)_2$] and [NiL·$ZnBr_2$·$(3,5\text{-lutidine})_2$] using DFT based on B3LYP/genecp method and 6-31G(d)/LanL2dz basis sets (without scale)