Supporting information

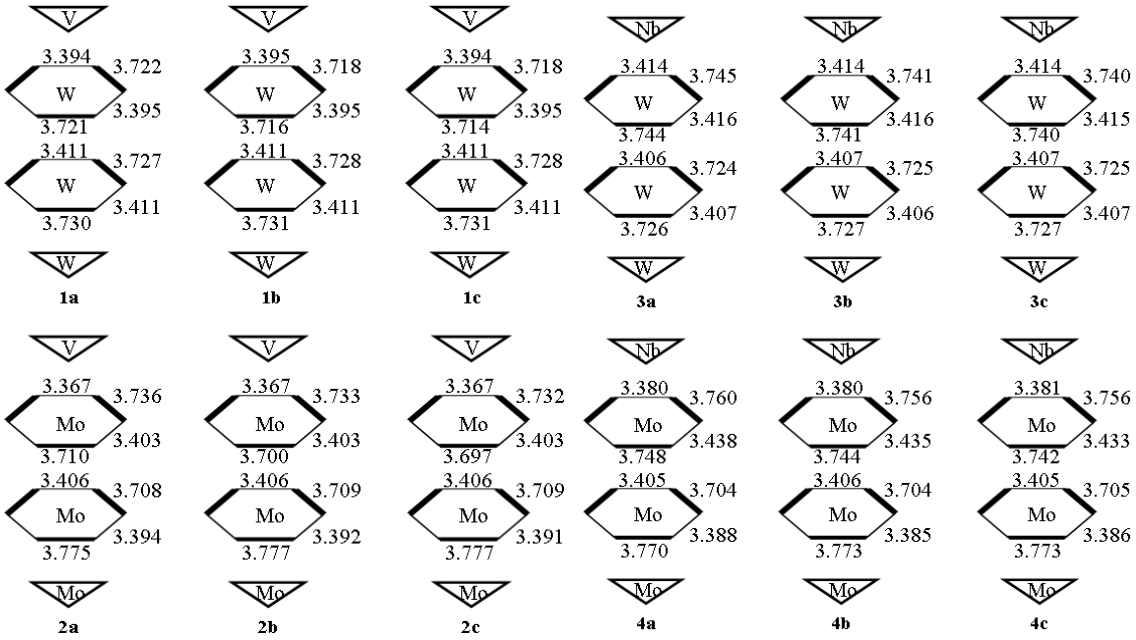
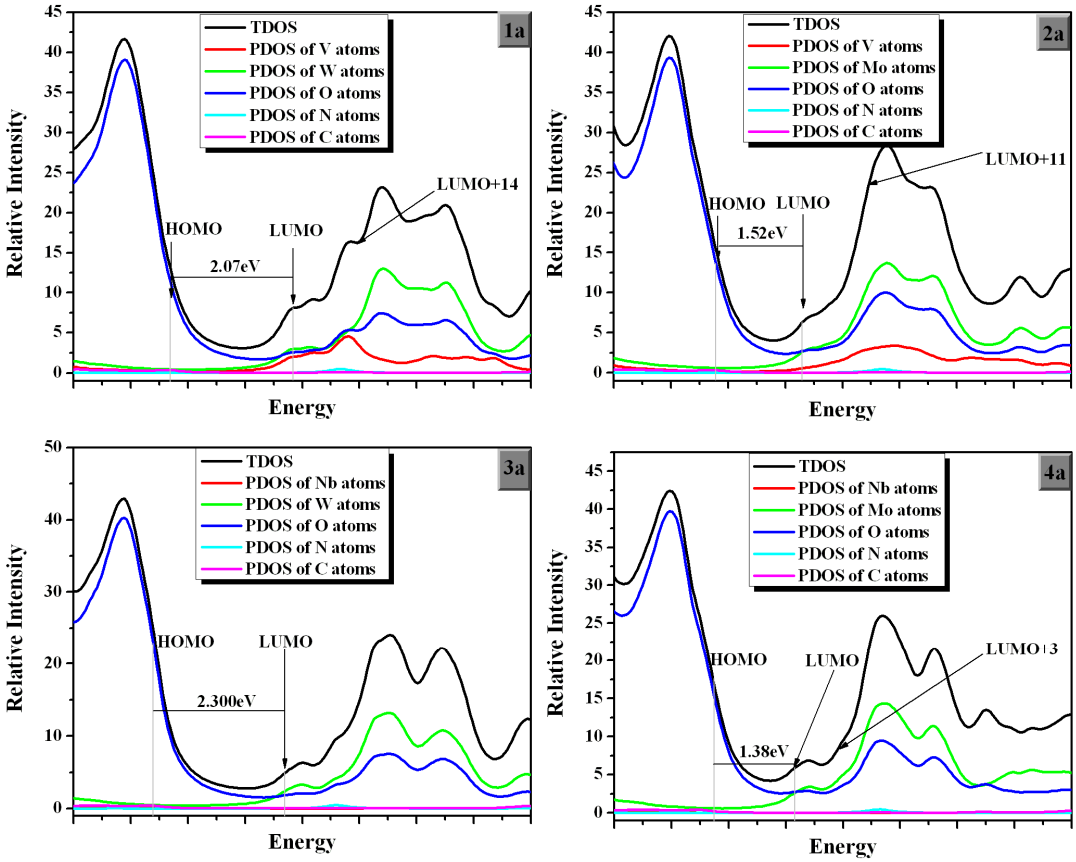


Figure S1. Alternation of W-W inside the two Belts of **a**, **b**, **c**, and **d** isomers at the BP86/TZP level



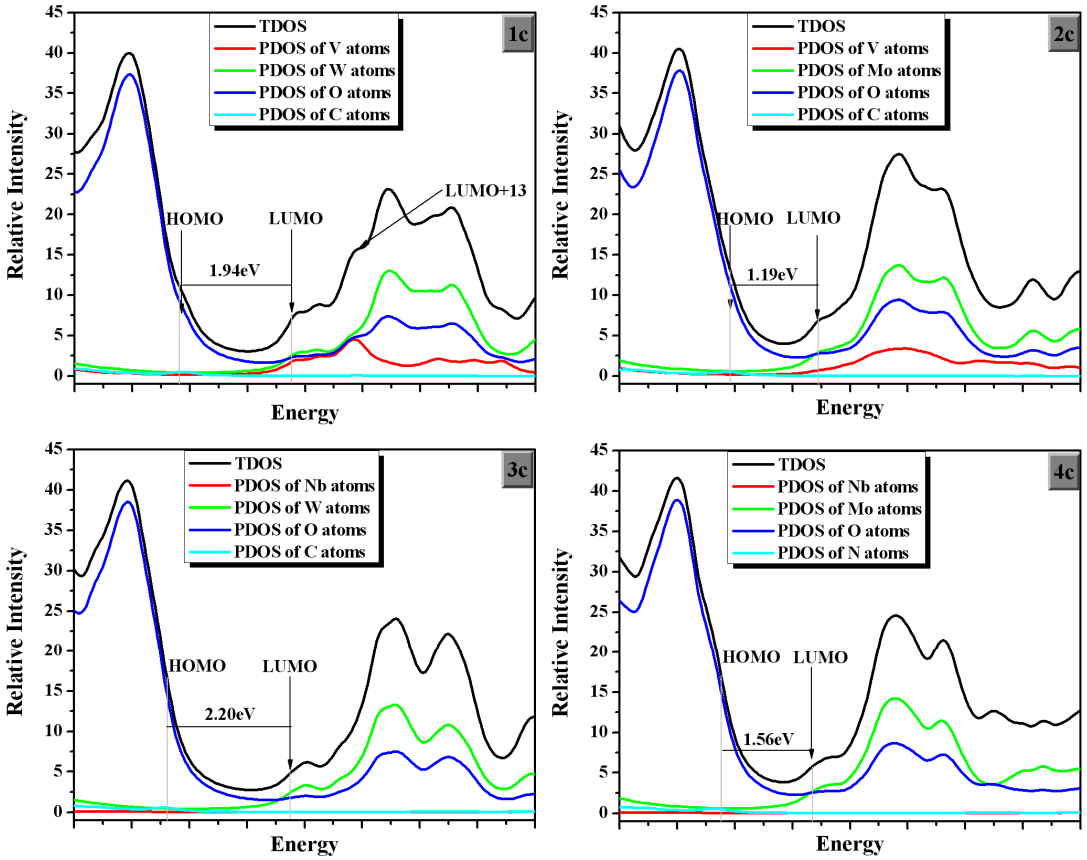


Figure S2. Partial Density of State (PDOS) of Series **a** and **c** Compounds

Table S1. SAOP/TZP Calculated Excited State Transition Energy (ΔE_{ge}, eV), Oscillator Strengths (f_{eg}), and Major Assignment of Optical Transitions for Series **a** and **c**

Systems	E_{ge}	f_{eg}	Major transition	
1a	2.693	0.024	409a" →410a"	56.03%
			473a'→474a'	38.81%
1c	2.422	0.021	470a' →471a'	47.70%
			405a' →406a'	44.04%
2a	2.607	0.007	282a" →292a"	61.56%
	2.584	0.005	351a' →353a'	70.84%
2c	2.389	0.010	348a' →350a'	94.05%
3a	3.308	0.009	421a" →422a"	63.92%
			486a' →490a'	12.27%
3c	3.238	0.004	409a" →418a"	56.01%
			412a" →418a"	35.85%
4a	2.300	0.003	298a" →304a"	76.01%
			296a" →304a"	21.96%
	2.372	0.003	365a' →367a'	63.22%
			296a" →304a"	15.81%
			302a" →305a"	9.46%
4c	2.542	0.006	357a" →300a"	77.60%