Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Quantum chemical studies on the enantiomerization mechanism of several $[Zn(py)_3(tach)]^{2+}$ derivates

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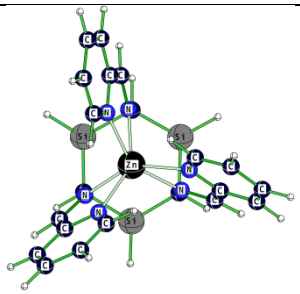	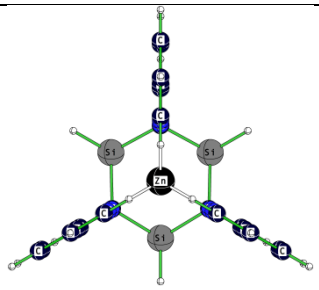
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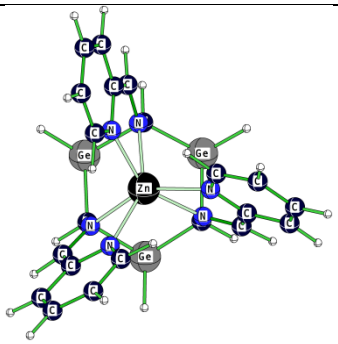	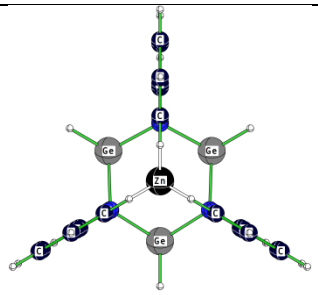
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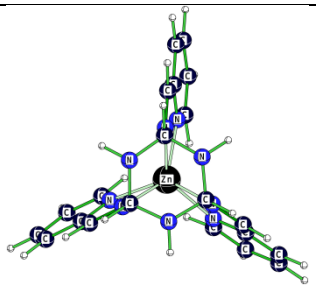
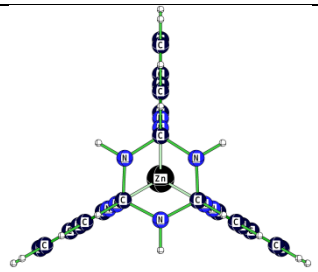
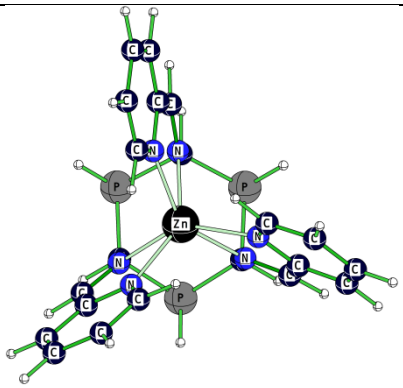
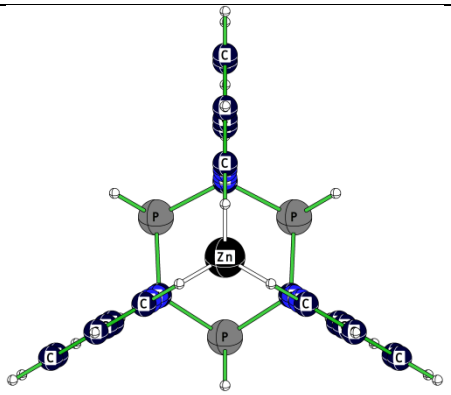
	
(C) (GS)	(TS)

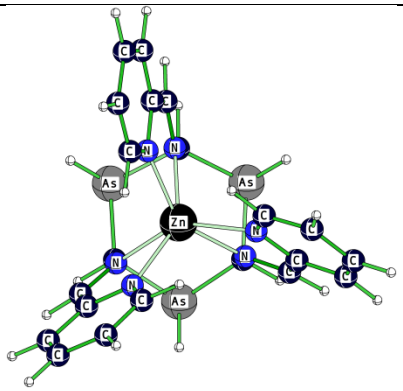
Figure S1. Calculated structures (B3LYP/LANL2DZp) of the ground (GS) and transition (TS) state of $[Zn(py_3tach\text{-}X)]^{2+}$ during the enantiomerization process.
(A): X = Si, (B): X = Ge and (C): X = N .



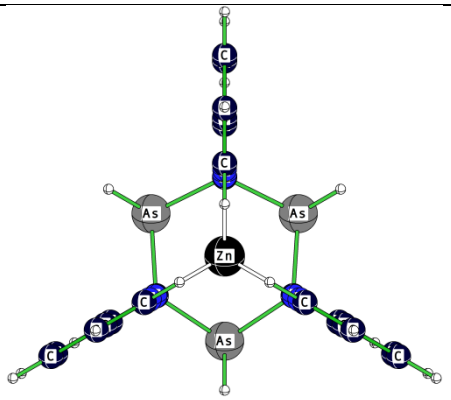
(A) GS



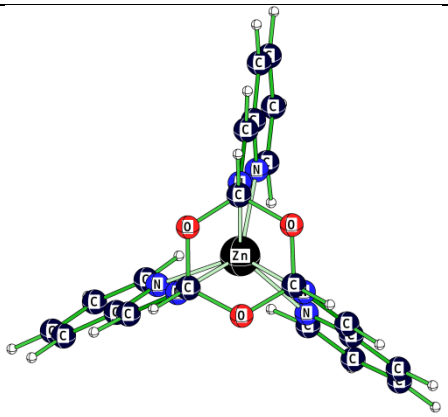
TS



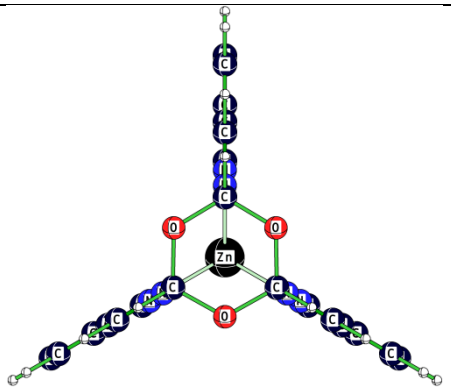
(B) GS



TS

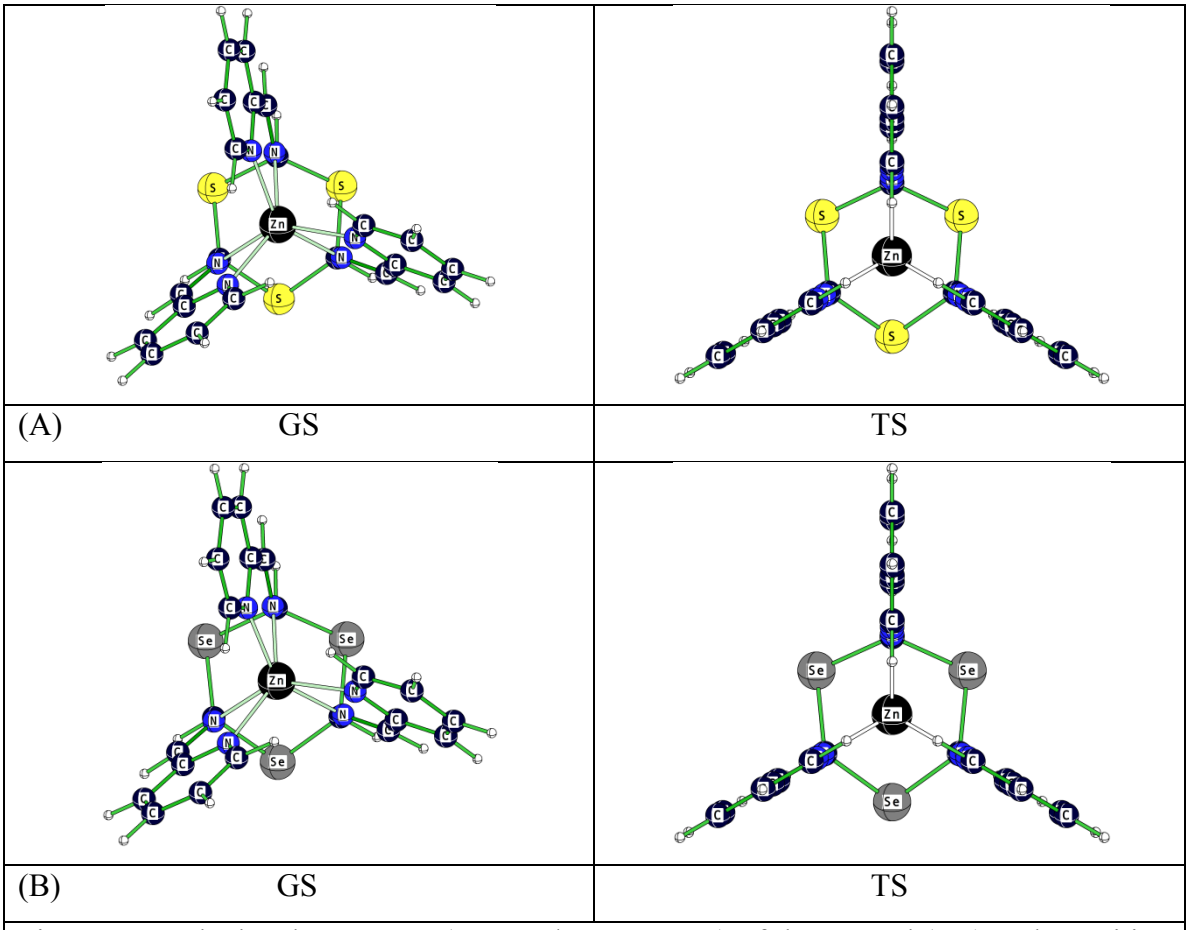


(C) GS



TS

Figure S2. Calculated structures (B3LYP/LANL2DZp) of the ground (GS) and transition (TS) state of $[Zn(py_3tach\text{-}X)]^{2+}$ during the enantiomerization process.
(A): X = P; (B): X = As and (C): X = O.



(A) GS	TS
(B) GS	TS

Figure S3. Calculated structures (B3LYP/LANL2DZp) of the ground (GS) and transition (TS) state of $[Zn(py_3tach\text{-}X)]^{2+}$ during the enantiomerization process.

(A): X = S; (B): X = As (Se).

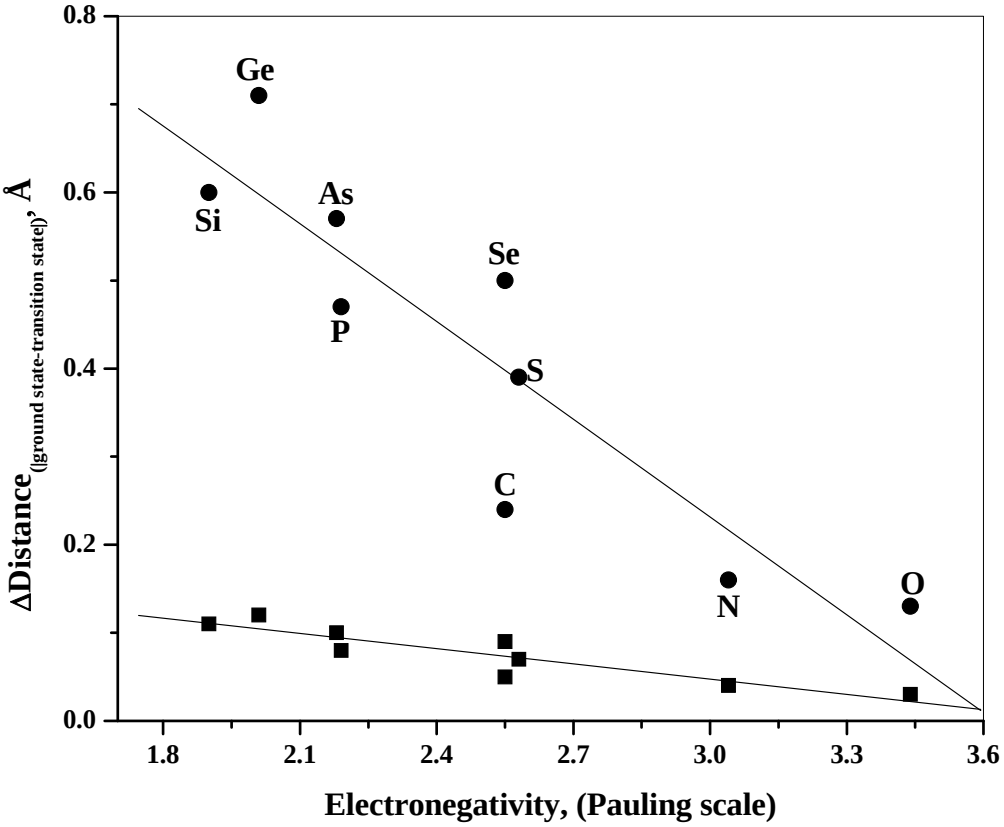


Figure S4**.** Calculated (RB3LYP/LANL2DZp) Δ distance for the ground and transition states of the complexes $[Zn(py_3tach\text{-}X)]^{2+}$ (X = C, Si, Ge, N, P, As O, S and Se) versus electronegativity (Pauling scale).

●: $\Delta(H_{py}\text{---}H_{py})$, ■: $\Delta(N_{py}\text{---}N_{py})$.

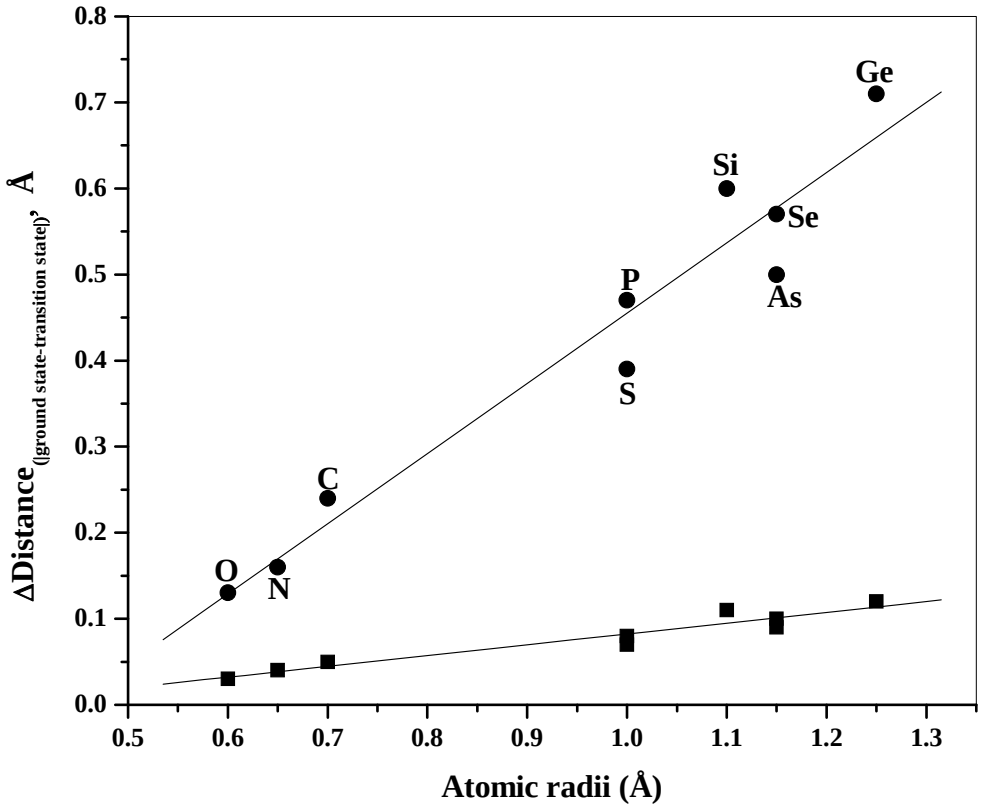


Figure S5**.** Calculated (RB3LYP/LANL2DZp) Δ difference for the ground and transition state of the complexes $[Zn(py_3tach\text{-}X)]^{2+}$ (X = C, Si, Ge, N, P, As O, S and Se) versus atomic size (Å).

●: $\Delta(H_{py}\text{---}H_{py})$, ■: $\Delta(N_{py}\text{---}N_{py})$.