

## Supplementary Information

**Table S1** Relative energies (B3LYP/LANL2DZ in eV) and relative abundances (%) for the  $\text{Pt}(\text{CN})_6^{2-}\cdot\text{M}_2$  and  $\text{Pt}(\text{CN})_4^{2-}\cdot\text{M}_2$  M = Ad, Cy, Th, Ur complexes.

**Figure S1** Geometric structures of the two conformers (B3LYP/LANL2DZ) of a)  $\text{Pt}(\text{CN})_6^{2-}\cdot\text{Ad}$ , b)  $\text{Pt}(\text{CN})_6^{2-}\cdot\text{Cy}$ , c)  $\text{Pt}(\text{CN})_6^{2-}\cdot\text{Th}$ , and d)  $\text{Pt}(\text{CN})_6^{2-}\cdot\text{Ur}$  labelled **I** and **II**. Relative energies (eV) for the two isomers are displayed.

**Figure S2** Geometric structures of the two conformers (B3LYP/LANL2DZ) of a)  $\text{Pt}(\text{CN})_4^{2-}\cdot\text{Ad}$ , b)  $\text{Pt}(\text{CN})_4^{2-}\cdot\text{Cy}$ , c)  $\text{Pt}(\text{CN})_4^{2-}\cdot\text{Th}$ , and d)  $\text{Pt}(\text{CN})_4^{2-}\cdot\text{Ur}$  labelled **I** and **II**. Relative energies (eV) for the two isomers are displayed.

**Figure S3** Geometric structures of the three conformers (B3LYP/LANL2DZ) of a)  $\text{Pt}(\text{CN})_6^{2-}\cdot\text{Ad}_2$ , b)  $\text{Pt}(\text{CN})_6^{2-}\cdot\text{Cy}_2$ , c)  $\text{Pt}(\text{CN})_6^{2-}\cdot\text{Th}_2$ , and d)  $\text{Pt}(\text{CN})_6^{2-}\cdot\text{Ur}_2$  labelled **I** and **II**. Relative energies (eV) for the two isomers are displayed.

**Figure S4** Geometric structures of the three conformers (B3LYP/LANL2DZ) of a)  $\text{Pt}(\text{CN})_4^{2-}\cdot\text{Ad}_2$ , b)  $\text{Pt}(\text{CN})_4^{2-}\cdot\text{Cy}_2$ , c)  $\text{Pt}(\text{CN})_4^{2-}\cdot\text{Th}_2$ , and d)  $\text{Pt}(\text{CN})_4^{2-}\cdot\text{Ur}_2$  labelled **I** and **II**. Relative energies (eV) for the two isomers are displayed.

**Table S1: Relative energies (eV)<sup>a</sup> and relative abundances (%) for the Pt(CN)<sub>6</sub><sup>2-</sup>·M<sub>2</sub> and Pt(CN)<sub>4</sub><sup>2-</sup>·M<sub>2</sub> M = Ad, Cy, Th, Ur complexes.<sup>a,b</sup>**

	Relative Energies			Relative Abundances		
	I	II	III	I	II	III
<b>Pt(CN)<sub>6</sub><sup>2-</sup>·M<sub>2</sub></b>						
Adenine	0	0.012	0.078	59.8	37.3	2.9
Uracil	0	0.006	0.592	56.1	43.9	0.0
Thymine	0	0.060	0.598	91.0	9.0	0.0
Cytosine	0	0.080	0.164	95.6	4.2	0.2
<b>Pt(CN)<sub>4</sub><sup>2-</sup>·M<sub>2</sub></b>						
Adenine	0	0.021	0.170	69.4	30.5	0.1
Uracil	0	0.091	0.411	89.9	10.1	0.0
Thymine	0	0.105	0.870	98.3	1.7	0.0
Cytosine	0	0.091	0.411	97.1	2.9	0.0

<sup>a</sup> Relative energies calculated at the B3LYP/ LANL2DZ level of theory.

<sup>b</sup> Relative abundances calculated using the Boltzmann distribution and T=373K.

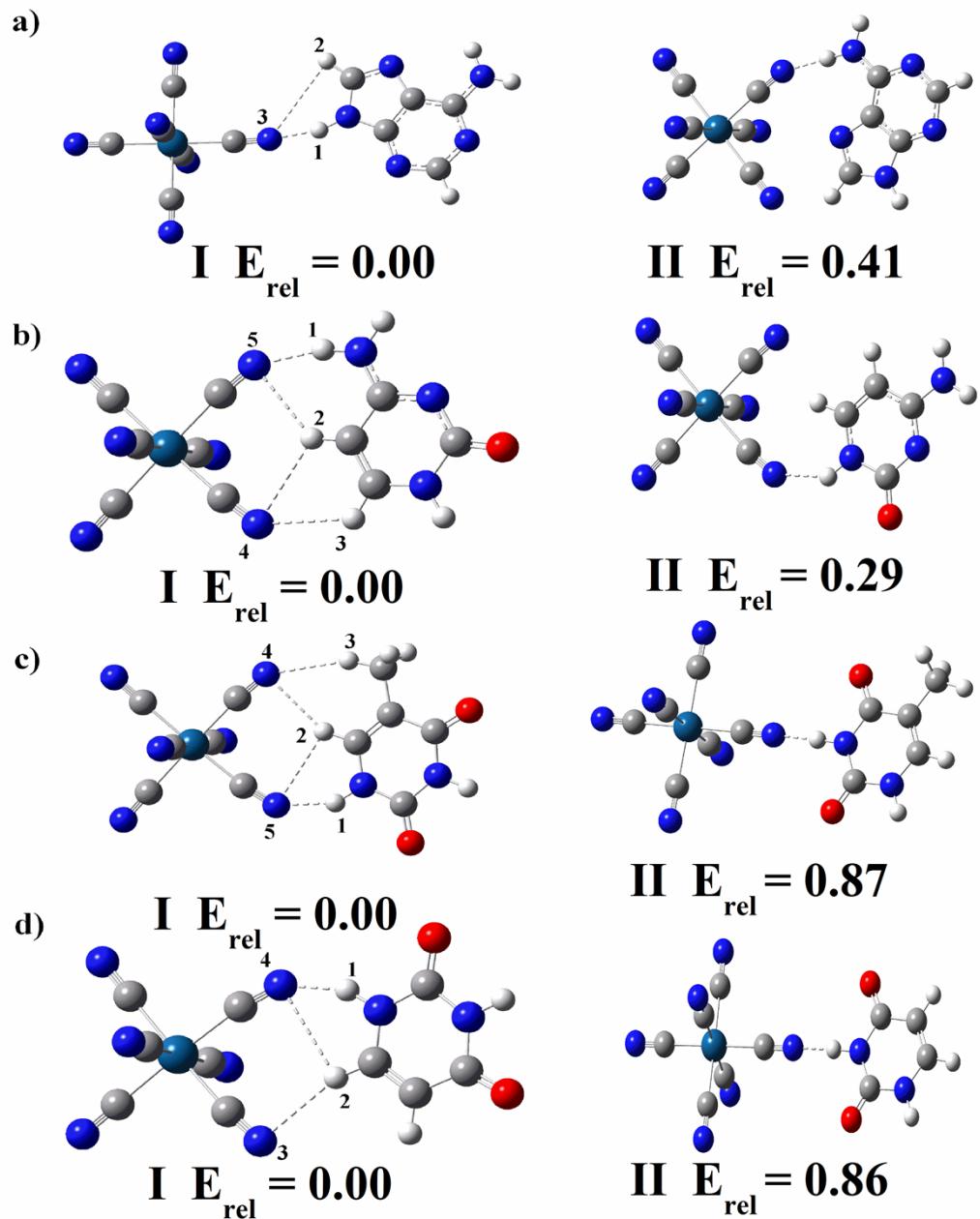


Fig. S1

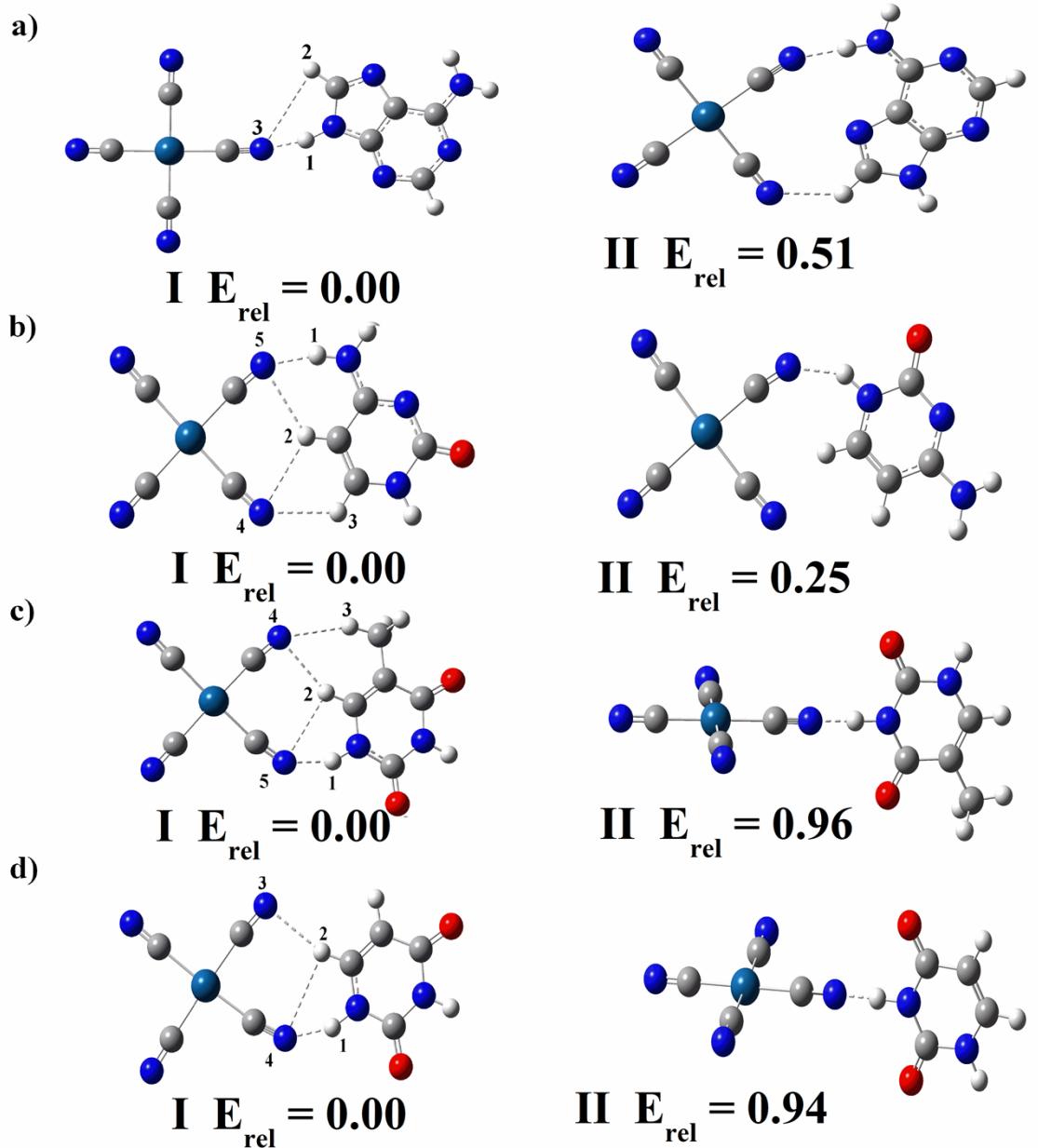
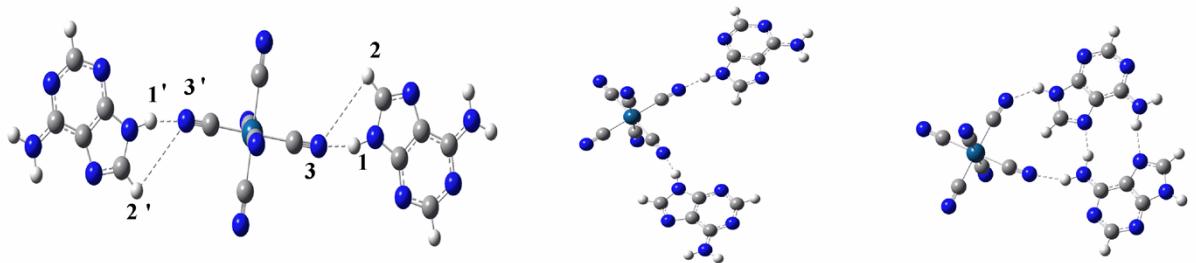
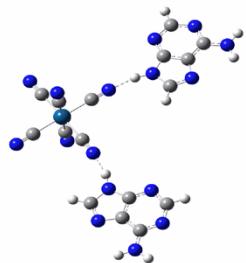


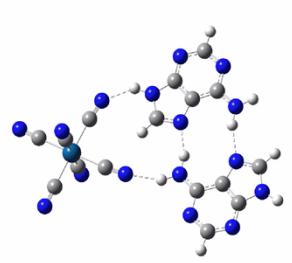
Fig. S2



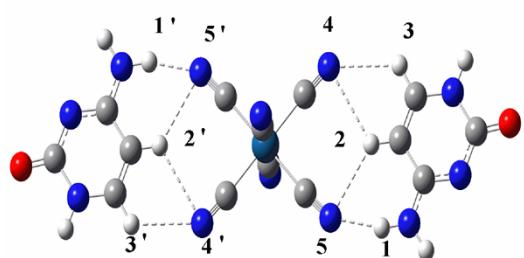
I  $E_{\text{rel}} = 0.00$



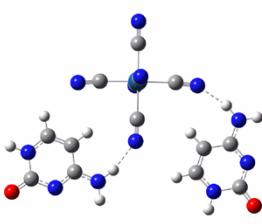
II  $E_{\text{rel}} = 0.01$



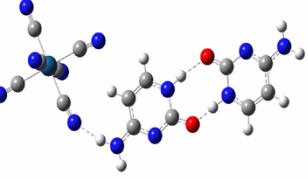
III  $E_{\text{rel}} = 0.08$



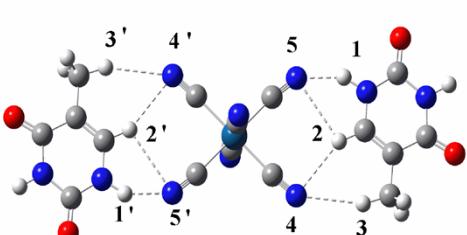
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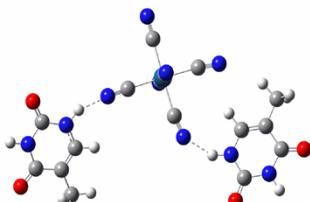
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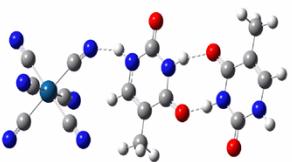
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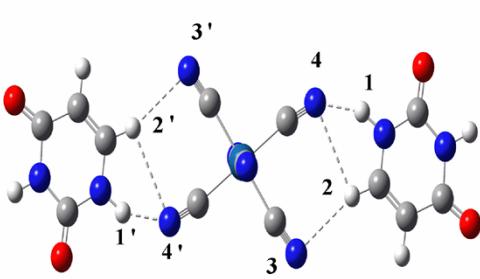
I  $E_{\text{rel}} = 0.00$



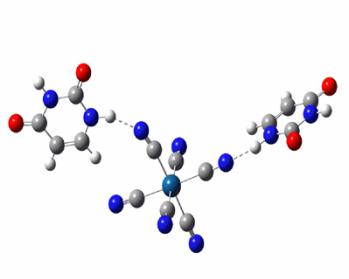
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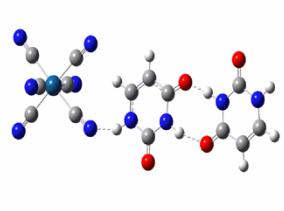
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I  $E_{\text{rel}} = 0.00$

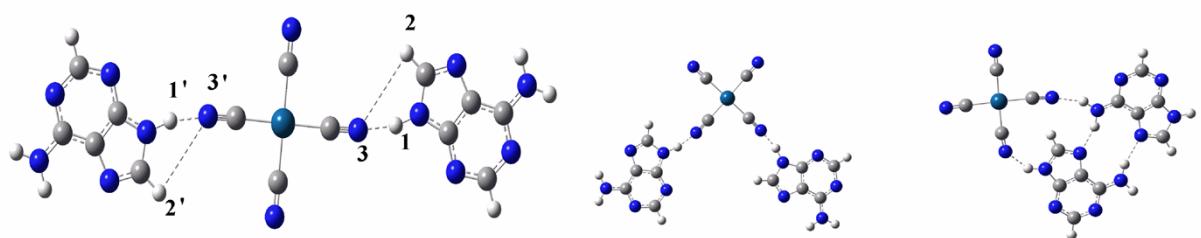


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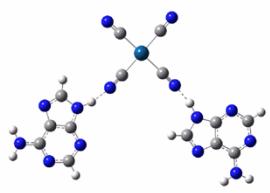


III  $E_{\text{rel}} = 0.59$

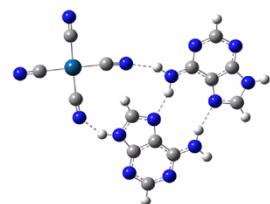
Fig. S3



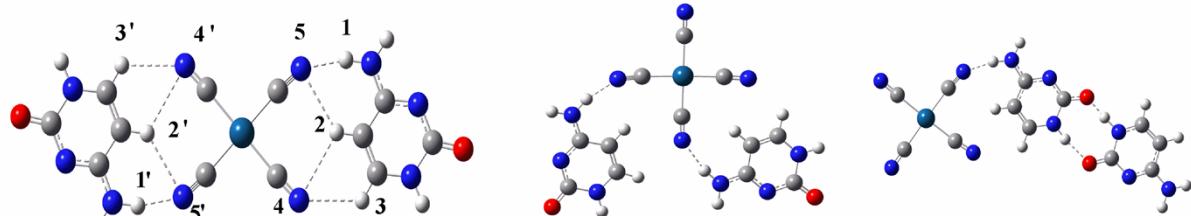
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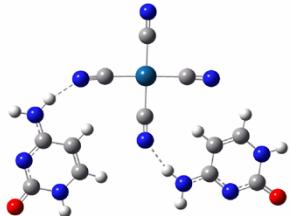
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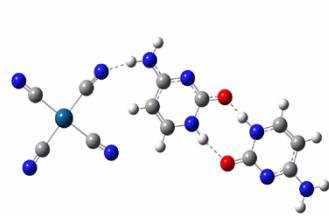
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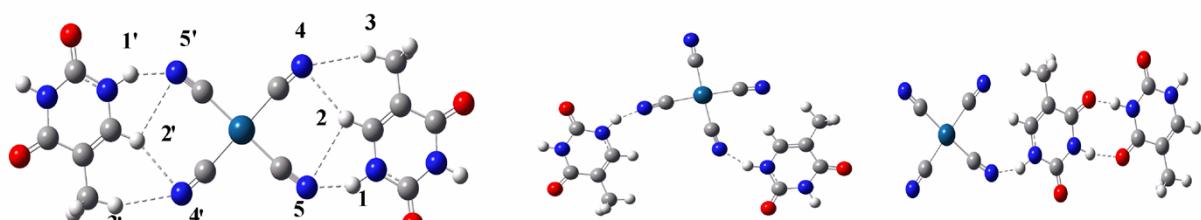
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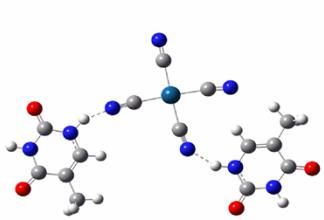
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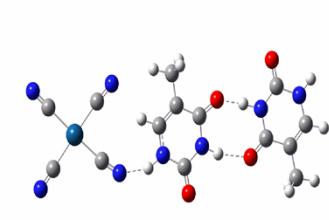
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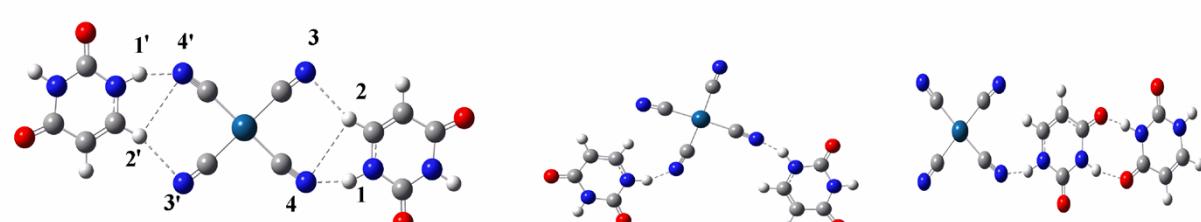
I  $E_{\text{rel}} = 0.00$



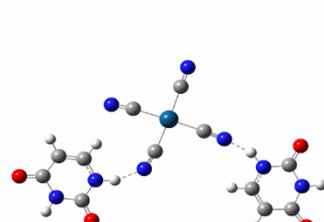
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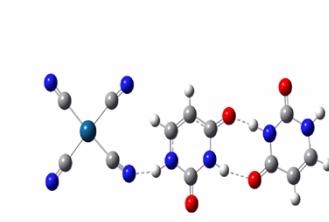
III  $E_{\text{rel}} = 0.87$



I  $E_{\text{rel}} = 0.00$



II  $E_{\text{rel}} = 0.06$



III  $E_{\text{rel}} = 0.86$

Fig. S4