Supplementary data for the article:

Malenov, D. P.; Hall, M. B.; Zarić, S. D. Influence of Metal Ion on Chelate–Aryl Stacking Interactions. *International Journal of Quantum Chemistry* **2018**, *118* (16). https://doi.org/10.1002/qua.25629

Potential energy curves in additional orientations

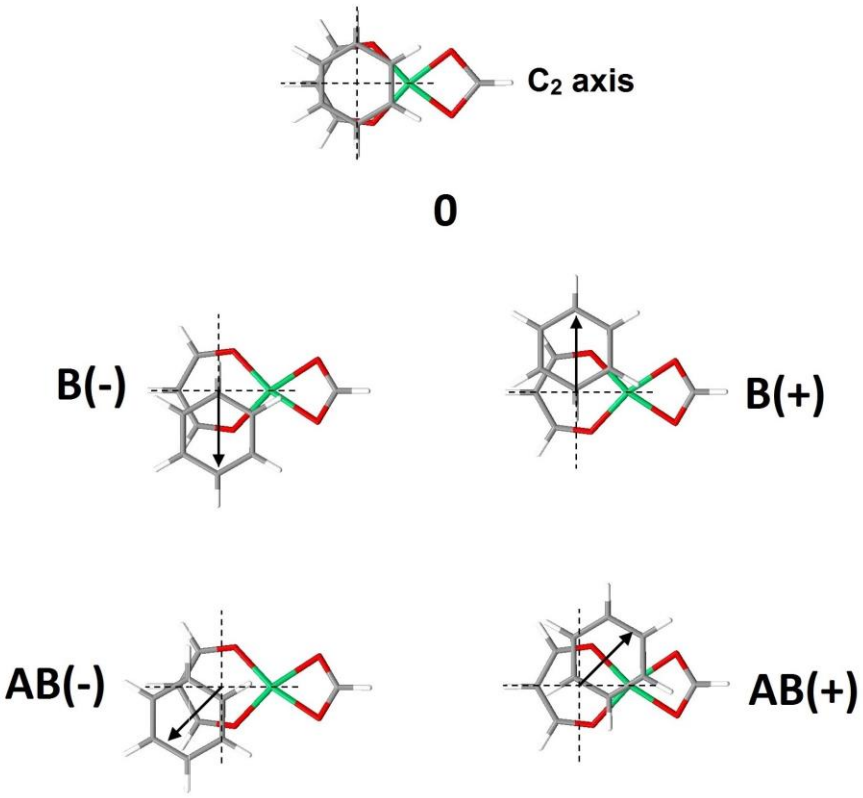

Figure S1. Additional model systems for calculations of chelate-aryl potential energy surfaces

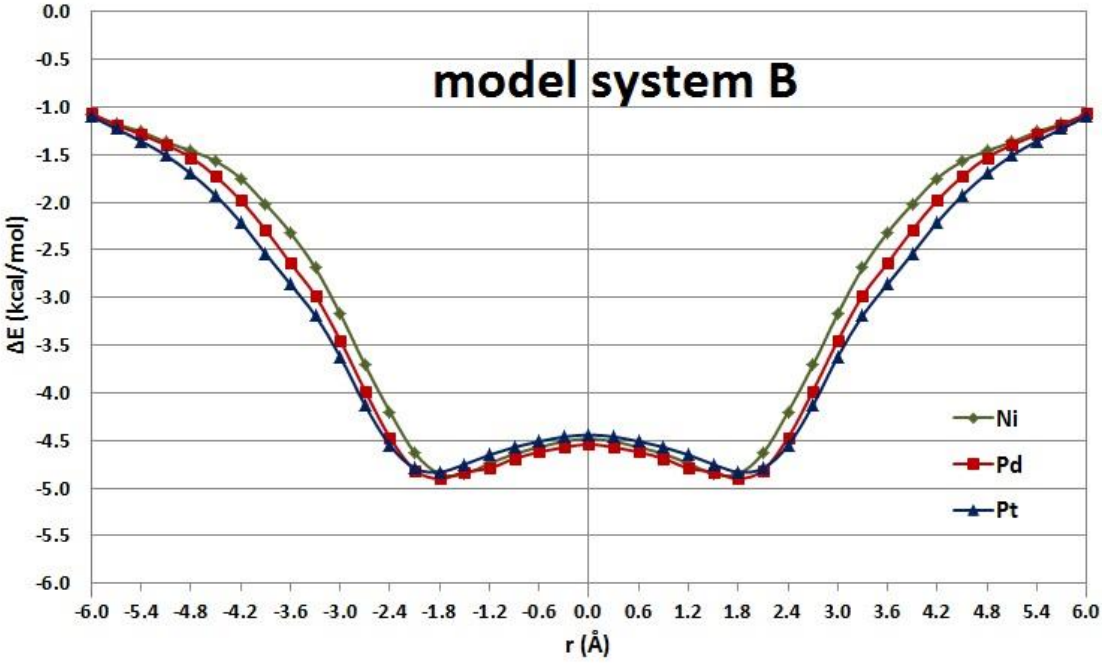

Figure S2. Potential energy curves for chelate-aryl stacking in model system B, calculated at M06-D3/def2-TZVP level. The calculations were performed on a series of geometries by changing the normal distances for a range of offset values; the curves present the energies of strongest interactions at all offset values.

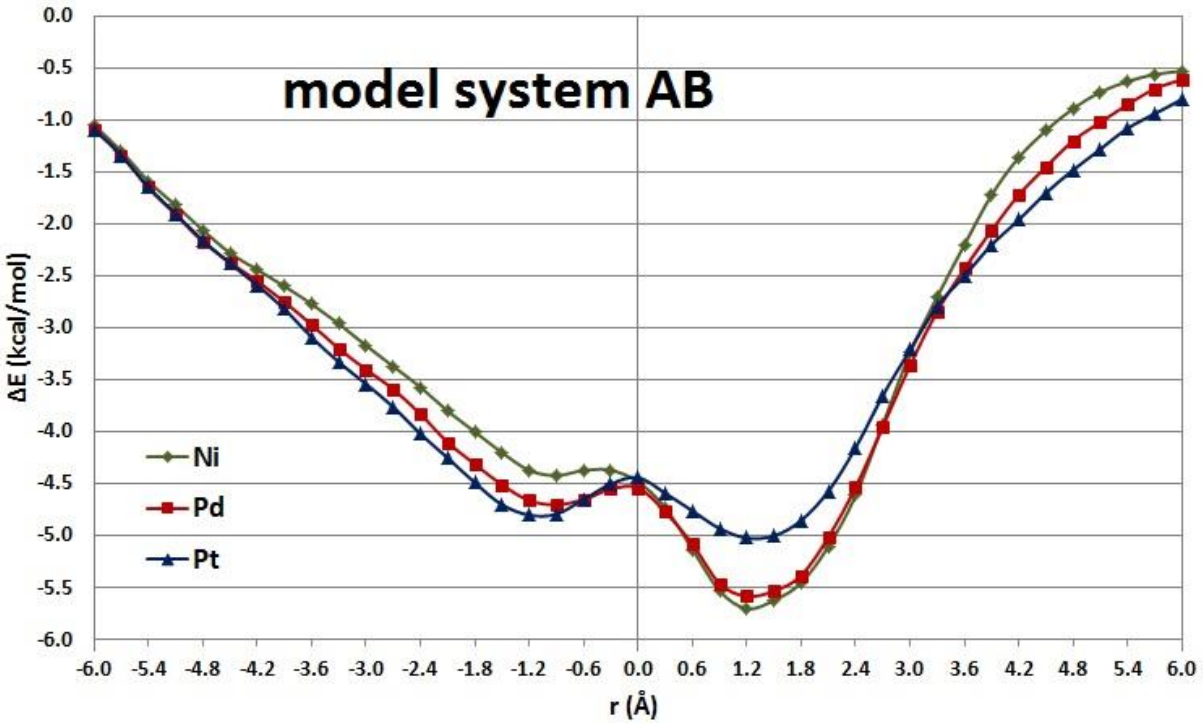

Figure S3. Potential energy curves for chelate-aryl stacking in model system AB, calculated at M06-D3/def2-TZVP level. The calculations were performed on a series of geometries by changing the normal distances for a range of offset values; the curves present the energies of strongest interactions at all offset values.

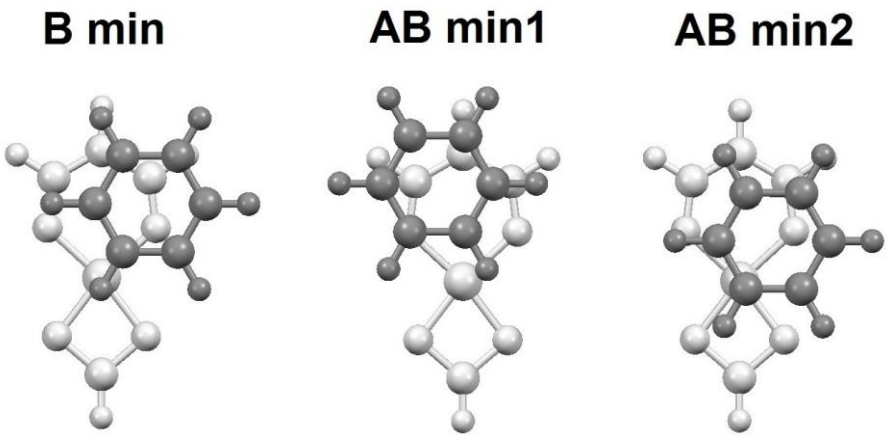

Figure S4. The parallel displaced energy minima on potential energy curvea B and AB for chelate-aryl stacking

Table S1. M06-D3/def2-TZVP interaction energies and correlation energies calculated as the difference between MP2 and HF energies with cc-pVTZ basis set for the minima on B and AB potential energy curves for chelate-aryl stacking interactions

	interaction energy M06-D3/def2-TZVP [kcal/mol]			correlation energy (MP2 – HF)/cc-pVTZ [kcal/mol]		
geometry	Ni	Pd	Pt	Ni	Pd	Pt
B min	-4.85	-4.90	-4.83	-7.52	-8.31	-8.46
AB min1	-4.42	-4.70	-4.80	-6.96	-7.55	-7.66
AB min2	-5.70	-5.58	-5.02	-7.63	-7.52	-8.66

Optimal normal distances for chelate-aryl stacking

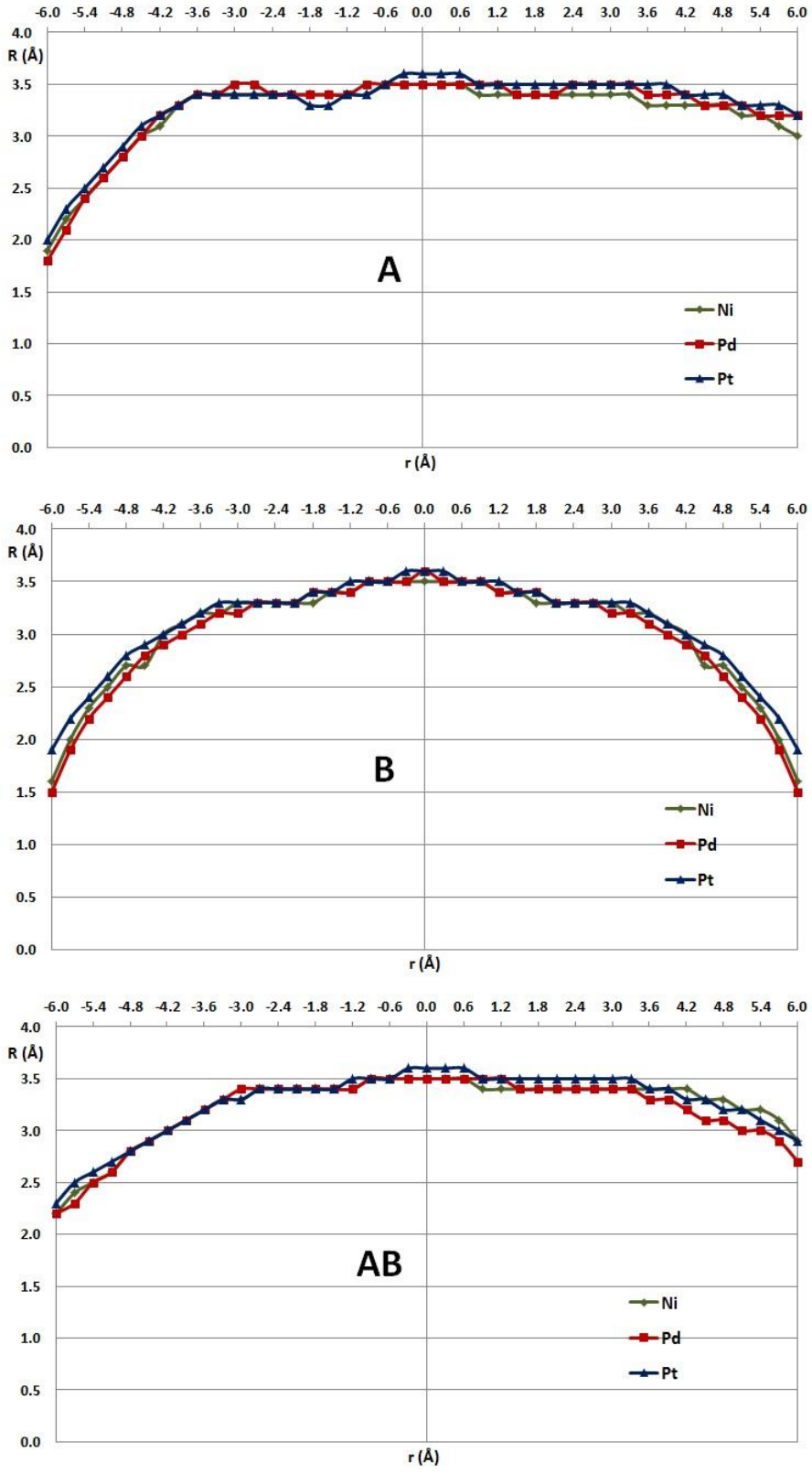

Figure S5. Optimal normal distances for chelate-aryl stacking