Electronic Supplementary Information

Paving the way for the synthesis of a series of divalent actinide complexes: A theoretical perspective

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Table S1 The relative energies (E_{re}, kcal/mol) of the different spin states (S) for the complex $[AnCp'_3]^-$ (An=Th-Am) at the BP86//ECP60MWB-SEG/6-31+G(d) level of theory.

$[AnCp'_3]^-$	S	E_{re}
$[ThCp'_3]^-$	1	0
	3	11.38
$[PaCp'_3]^-$	4	0
	2	0.34
$[UCp'_3]^-$	5	0
	3	4.36
$[NpCp'_3]^-$	6	0
	4	7.64
	2	30.97
$[PuCp'_3]^-$	7	0
	5	11.72
	3	42.60
	1	80.75
$[AmCp'_3]^-$	8	0
	6	32.33
	4	85.67

Table S2 The total electronic energies (au) of the complexes $[AnCp'_3]^-$ and $AnCp'_3$ at the BP86//ECP60MWB-SEG/6-31+G(d) level of theory in THF solution.

	$AnCp'_3$	$[AnCp'_3]^-$
Th	-2214.59752	-2214.648778
Pa	-2248.31828	-2248.371594
U	-2283.84485	-2283.904000
Np	-2321.39761	-2321.455945
Pu	-2360.88971	-2360.958261
Am	-2402.44211	-2402.533794