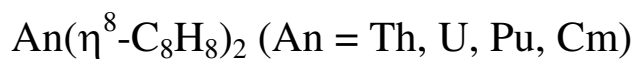


Are the ground states of the later actinocenes multiconfigurational?

All-electron spin-orbit coupled CASPT2 calculations on



Andrew Kerridge and Nikolas Kaltsoyannis*

Supporting Information

SOC State	Contribution from SOF state (%)				
	¹ A _g	¹ A _u	¹ B _{1u}	³ A _u	³ B _{1u}
1	100.0	0.0	0.0	0.0	0.0
2	0.0	98.6	0.0	0.0	1.4
3	0.0	0.0	98.6	1.4	0.0
4	0.0	0.0	0.0	73.1	26.9
5	0.0	0.0	0.0	26.9	73.1

Table s1. Percentage contribution from ThCOT₂ SOF states to the low-lying SOC states, as illustrated in Figure 3.

SOC State	Contribution from SOF state (%)							
	³ A _g	³ B _{1g}	³ A _g	³ B _{1g}	³ B _{2g}	³ B _{3g}	¹ A _g	¹ B _{1g}
1	41.9	41.9	0.0	0.0	0.0	11.4	0.0	0.0
2	41.9	41.9	0.0	0.0	11.4	0.0	0.0	0.0
3	0.0	0.0	0.0	34.4	24.8	24.8	14.5	0.0
4	0.0	0.0	34.4	0.0	24.8	24.8	0.0	14.5
5	88.3	0.0	0.0	0.0	4.4	4.4	0.0	0.0
6	0.0	88.3	0.0	0.0	4.4	4.4	0.0	0.0
7	0.0	0.0	45.7	52.8	0.0	0.0	0.0	0.0
8	0.0	0.0	45.7	52.8	0.0	0.0	0.0	0.0

Table s2. Percentage contribution from UCOT₂ SOF states to the low-lying SOC states, as illustrated in Figure 5.

SOC State	Contribution from SOF state (%)						
	5A_g	$^5B_{2g}$	$^5B_{3g}$	$^5B_{2g}$	$^5B_{3g}$	5A_g	$^5B_{1g}$
1	49.7	19.5	19.5	0.0	0.0	0.0	0.0
2	49.5	32.5	4.3	0.0	2.5	0.0	0.0
3	49.5	4.3	32.5	2.5	0.0	0.0	0.0
4	5.6	1.8	0.0	42.3	43.9	0.0	0.0
5	5.6	0.0	1.8	43.9	42.3	0.0	0.0
6	49.7	17.3	17.3	2.6	2.6	0.0	0.0
7	49.3	15.4	15.4	4.7	4.7	0.0	0.0

Table s3. Percentage contribution from PuCOT₂ SOF states to the low-lying SOC states, as illustrated in Figure 7.

SOC State	Contribution from SOF state (%)	
	7A_g	$^7B_{1g}$
1	88.8	2.4
2	88.8	2.4
3	90.0	3.0
4	90.0	3.0
5	92.9	1.7
6	92.9	1.7
7	95.3	0.0
8	2.2	92.5
9	2.2	92.5

Table s4. Percentage contribution from CmCOT₂ SOF states to the low-lying SOC states, as illustrated in Figure 9.