Electronic Supplementary Material (ESI) for Dalton Transactions

Supplementary Material

Modeling the properties of lanthanoid single-ion magnets using an effective point-charge approach

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Energy (cm^{-1})	Wave function			
0	**1.00|-5>**	0.01·|-1>		
0	0.01·|1>	**1.00|5>**		
25	**0.71·|-6>**	0.39·|-2>	0.39·|2>	**0.71·|6>**
25	**0.71·|-6>**	0.37·|-2>	0.37·|2>	**0.71·|6>**
31	0.04·|-8>	**0.71·|-4>**	**0.71·|4>**	0.04·|8>
31	0.04·|-8>	**0.70·|-4>**	**0.70·|4>**	0.04·|8>
89	**0.79·|-7>**	0.61·|-3>	0.01·|1>	
89	0.01·|-1>	0.61·|3>	**0.79·|7>**	
110	0.61·|-7>	**0.79·|-3>**	0.02·|1>	
110	0.02·|-1>	**0.79·|3>**	0.61·|7>	
162	**0.92|-8>**	0.06|-4>	0.06|4>	0.39|8>
162	0.39|-8>	0.02|-4>	0.06|4>	**0.92|8>**
179	0.04·|-6>	**0.71·|-2>**	**0.71·|2>**	0.04·|6>
190	0.04·|-6>	**0.71·|-2>**	**0.71·|2>**	0.04·|6>
247	0.02·|-5>	**1.00|-1>**	0.03·|3>	
247	0.03·|-3>	**1.00|1>**	0.02·|5>	
270	**1.00|0>**			

Table S.1: Energies and modulus of the contribution of each M_J to the wave-functions of the ground state multiplets of $HoPc_2$

Energy (cm^{-1})	Wave function			
0	0.01·|-9/2>	**1.00·|-1/2>**	0.01·|7/2>	
0	0.01·|-7/2>	**1.00·|1/2>**	0.01·|9/2>	
58	0.05·|-11/2>	**1.00·|-3/2>**	0.06·|5/2>	0.01·|13/2>
58	0.01·|-13/2>	0.06·|5/2>	**1.00·|3/2>**	0.05·|11/2>
79	**1.00·|-15/2>**	0.06·|-7/2>		
79	0.06·|7/2>	**1.00·|15/2>**		
129	**0.89·|-13/2>**	0.46·|-5/2>	0.04·|3/2>	
129	0.04·|-3/2>	0.46·|5/2>	**0.89·|13/2>**	
159	0.46·|-13/2>	**0.89·|-5/2>**	0.04·|3/2>	
159	0.04·|-3/2>	**0.89·|5/2>**	0.46·|13/2>	
234	**1.00·|-11/2>**	0.05·|-3/2>		
234	0.05·|-3/2>	**1.00·|11/2>**		
240	0.06·|-13/2>	**1.00·|-7/2>**	0.01·|1/2>	
240	0.01·|-1/2>	**1.00·|7/2>**	0.06·|13/2>	
275	**1.00·|-9/2>**	0.01·|-1/2>		
275	0.01·|1/2>	**1.00·|9/2>**		

Table S.2: Energies and modulus of the contribution of each M_J to the wave-functions of the ground state multiplets of $ErPc_2$

Energy (cm^{-1})	Wave function			
0	0.01·|-4>	**1.00·|0>**	0.01·|4>	
3	**0.71·|-6>**	0.05·|-2>	0.05·|2>	**0.71·|6>**
3	**0.71·|-6>**	0.05·|-2>	0.05·|2>	**0.71·|6>**
18	0.01·|-5>	**1.00·|-1>**	0.05·|3>	
18	0.05·|-3>	**1.00·|1>**	0.01·|5>	
69	0.07·|-6>	**0.70·|-2>**	**0.70·|2>**	0.07·|6>
88	0.05·|-6>	**0.71·|-2>**	**0.71·|2>**	0.05·|6>
178	**1.00·|-3>**	0.05·|1>		
178	0.05·|-1>	**1.00·|3>**		
291	**0.71·|-4>**	**0.71·|4>**		
291	**0.71·|-4>**	**0.71·|4>**		
312	**1.00·|-5>**	0.01·|1>		
312	0.01·|-1>	**1.00·|5>**		

Table S.3: Energies and modulus of the contribution of each M_J to the wave-functions of the ground state multiplets of $TmPc_2$

Energy (cm^{-1})	Wave function	
0	**1.00·|-5/2>**	0.04·|3/2>
0	0.04·|-3/2>	**1.00·|5/2>**
224	**1.00·|-3/2>**	0.04·|5/2>
224	0.04·|-5/2>	**1.00·|3/2>**
366	**0.92·|-7/2>**	0.38·|1/2>
366	0.38·|-1/2>	**0.92·|7/2>**
372	0.38·|-7/2>	**0.92·|3/2>**
372	**0.92·|-3/2>**	0.38·|7/2>

Table S.4: Energies and modulus of the contribution of each M_J to the wave-functions of the ground state multiplets of $YbPc_2$