Electronic Supplementary Information for

Crystal structure diversity in the bis[hydrotris-(3,5-dimethylpyrazolyl)borate]iodouranium(III) complex; from neutral to cationic forms

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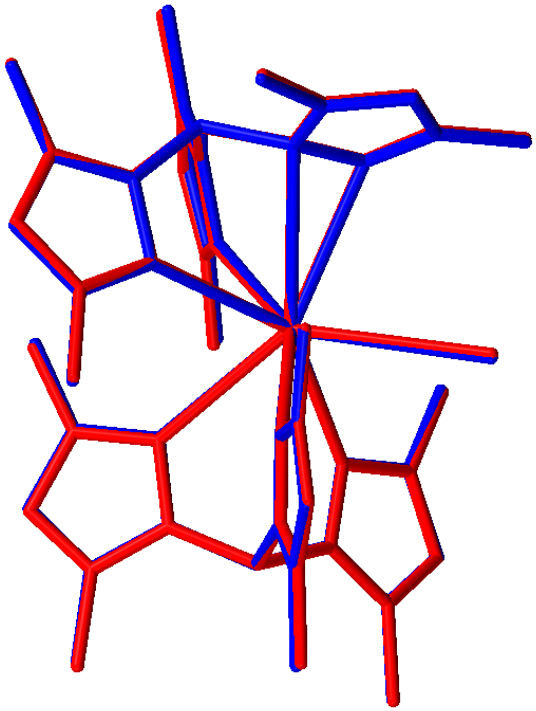

Figure SI1. Molecular Structures of [U(Tp^{Me2})$_2$I] at 296 K (red) and 150 K (blue).

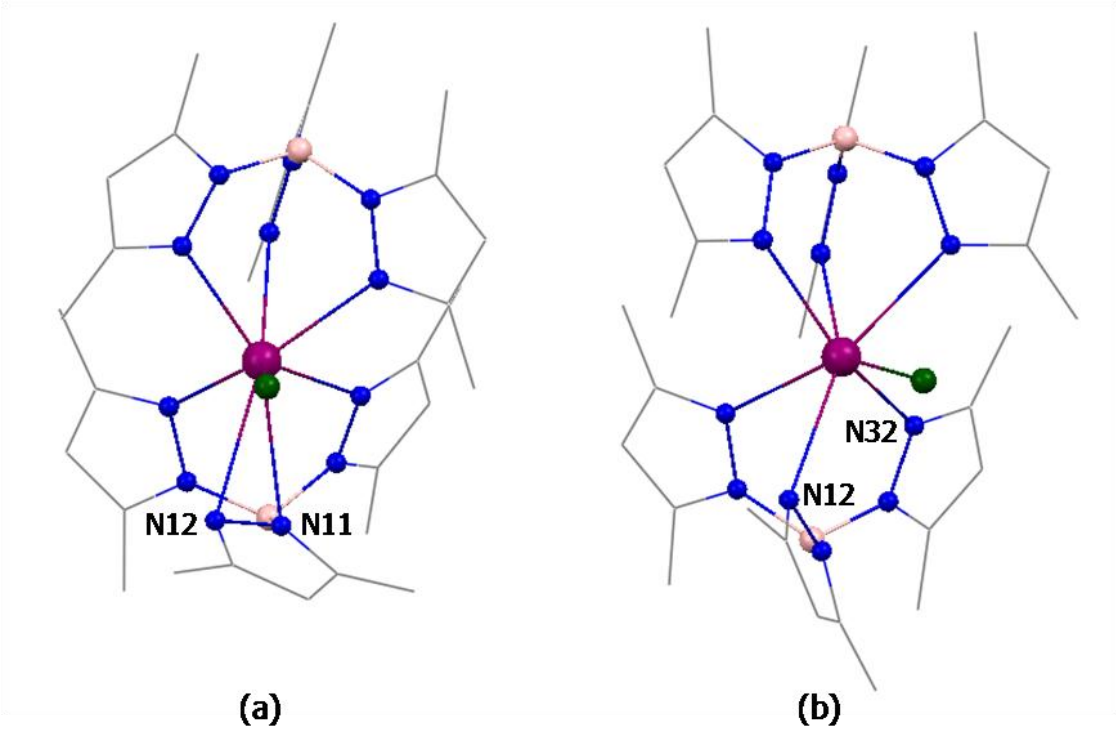

Figure SI2. Molecular Structures of Forms **1a** (a) and **1c** (b).

Table SI1. U–I Bond Lengths in Uranium(III) Complexes

Complex	d(U–I)/Å	Ref.	Complex	d(U–I)/Å	Ref.
$[U(Tp^{Me2})_2I]$, **1a**	3.2121(2)		$[U(Nacnac)_2I]$	3.0665(8)	7
$[U(Tp^{Me2})_2I]$, **1c**	3.1936(4)		$[U(Cp^{Me4,SiR3})_2I(THF)]$	3.0851(3)	8
$[U(TTCN)I_3(NCMe)_2]$	3.0872(3) 3.1489(3) 3.1544(3)	1	$[U(Cp^*)_2I(bipy)]$	3.2134(4)	9
$[U\{H_2B(pz^{tBu,Me})(pz^{Me,tBu})\}_2I]$	3.1027(11)	2	$[U(Cp^{tBu})I_2(py)_3]$	3.147(1) 3.191(1)	10
$[U\{H_2B(pz^{tBu,Me})(pz^{Me2})\}_2I]$	3.0989(9)	2	$[U(Cp^{tBu})_2I(py)_2]$	3.169(2) 3.172(2) 3.180(2)	10
$[U(Cp^*)_2I(NCMe)_2]$	3.2076(7)	3	$[U(BIPM^{TMS})I_2(THF)]$	3.1519(9) 3.173(1)	11
$[U(tpza)I_3(NCMe)]$	3.2383(14) 3.2637(10) 3.1632(10)	4	$[U(Cp^{Me4,Et})_2I\ (THF)]$	3.0929(4)	12
$[U(tpza)I_3(THF)]$	3.19114(6) 3.2087(7) 3.1439(6)	4	$[U(Cp^*)I_2(THF)_3]$	3.161(1) 3.162(1) 3.179(1) 3.168(1)	13
$[U(PNP)_2I]$	3.109(1)	5	$[UI_3(THF)_4]$	3.103(3) 3.168(2) 3.119(3)	14
$[U(PNP)I_2(^t\text{Bu-py})_2]$	3.106(1) 3.116(1)	5	$[U(tpa)I_3(py)]$	3.2612(7) 3.2944(7) 3.1893(7)	15
$[U\{H_2B(pz^{tBu,Me})_2\}I_2(THF)_2]$	3.104(2) 3.132(2)	6	$[UI_3(bipy)_2(py)]$	3.2032(9) 3.2073(8) 3.2511(8)	16
$[U\{H_2B(pz^{tBu,Me})_2\}I_2(OPPh_3)_2]$	3.164(2) 3.199(2)	6			

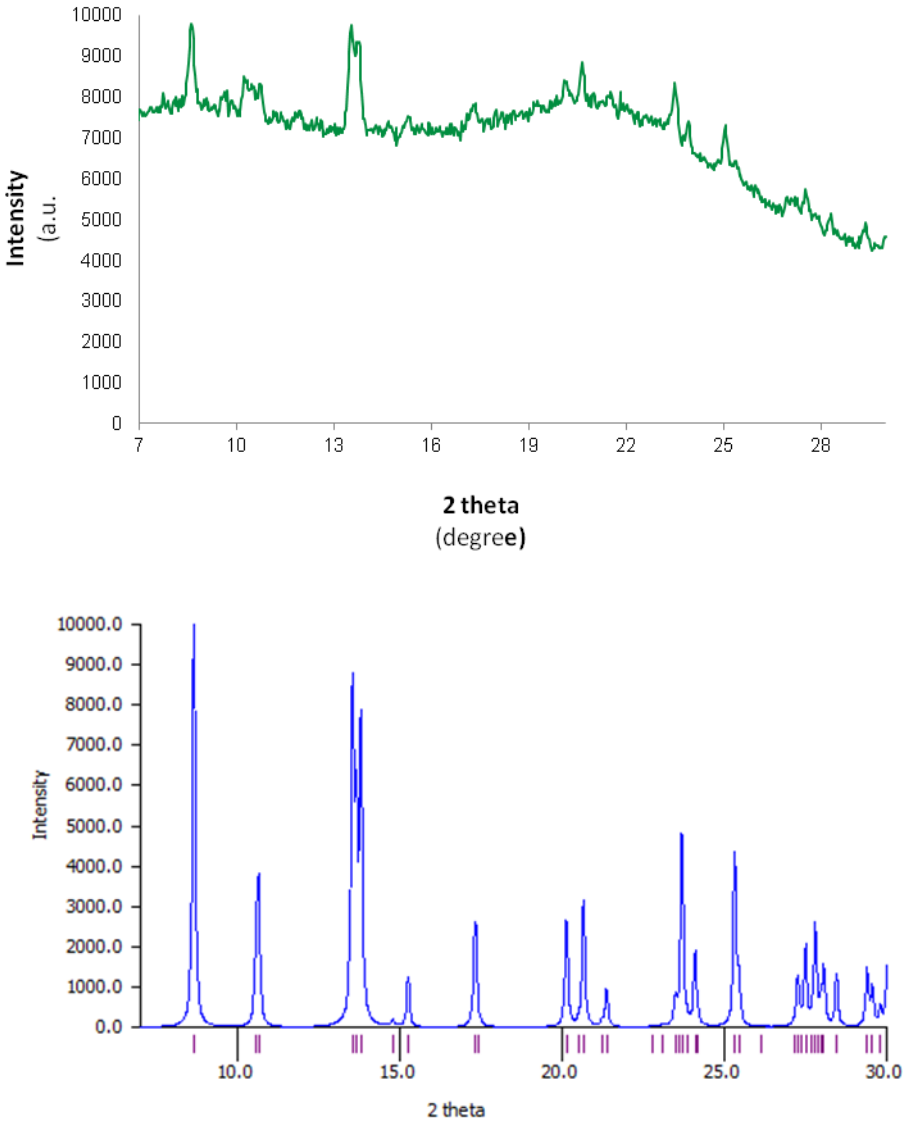

Figure SI3. Experimental powder X-ray diffractogram of the sample used for magnetic measurements (top) and powder X-ray diffractogram of **1b** simulated from the single crystal structure (bottom).

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