Electronic Supplementary Information

Two Rare Cr-Ln (Ln = Dy, Tb) Heterometallic Cluster Substituted Polyoxometalates Featuring Hexameric Aggregates: Hydrothermal Syntheses, Crystal Structures and Magnetic Studies

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Table S1 Selected bond lengths (Å) and valence bond summations (ΣS) for **1-Dy**.

Cr1			
Bond	Bond length(Å)	Bond valence	Sum of bond
Cr(1)-O(1)	1.938(7)	0.5216	ΣS = 2.831
Cr(1)-O(6)	1.941(7)	0.5167	
Cr(1)-O(2)	1.946(7)	0.5086	
Cr(1)-O(32)	1.995(7)	0.4353	
Cr(1)-O(39)	1.997(8)	0.4312	
Cr(1)-O(7)	2.008(7)	0.4177	
Dy1			
Bond	Bond length(Å)	Bond valence	Sum of bond
Dy(1)-O(11)	2.287(7)	0.5124	ΣS = 3.021
Dy(1)-O(8)	2.293(7)	0.5018	
Dy(1)-O(13)	2.335(7)	0.4440	
Dy(1)-O(1)	2.349(7)	0.4258	
Dy(1)-O(33)	2.457(7)	0.3085	
Dy(1)-O(31)	2.483(8)	0.2854	
Dy(1)-O(7)	2.492(7)	0.2779	
Dy(1)-O(32)	2.509(7)	0.2641	

Table S2 Selected bond lengths (Å) and valence bond summations (ΣS) for **1-Tb**.

Cr1			
Bond	Bond length(Å)	Bond valence	Sum of bond
Cr(1)-O(29)	1.934(6)	0.5250	ΣS = 2.864
Cr(1)-O(30)	1.941(6)	0.5167	
Cr(1)-O(27)	1.943(7)	0.5134	
Cr(1)-O(23)	1.981(6)	0.4551	
Cr(1)-O(8)	1.995(6)	0.4353	
Cr(1)-O(11)	2.008(6)	0.4190	
Tb1			
Bond	Bond length(Å)	Bond valence	Sum of bond
Tb(1)-O(20)	2.293(6)	0.5311	ΣS = 3.119
Tb(1)-O(6)	2.301(7)	0.5170	
Tb(1)-O(24)	2.343(6)	0.4561	
Tb(1)-O(29)	2.364(6)	0.4284	
Tb(1)-O(19)	2.463(6)	0.3188	
Tb(1)-O(18)	2.491(7)	0.2932	
Tb(1)-O(23)	2.498(6)	0.2872	
Tb(1)-O(11)	2.499(6)	0.2871	

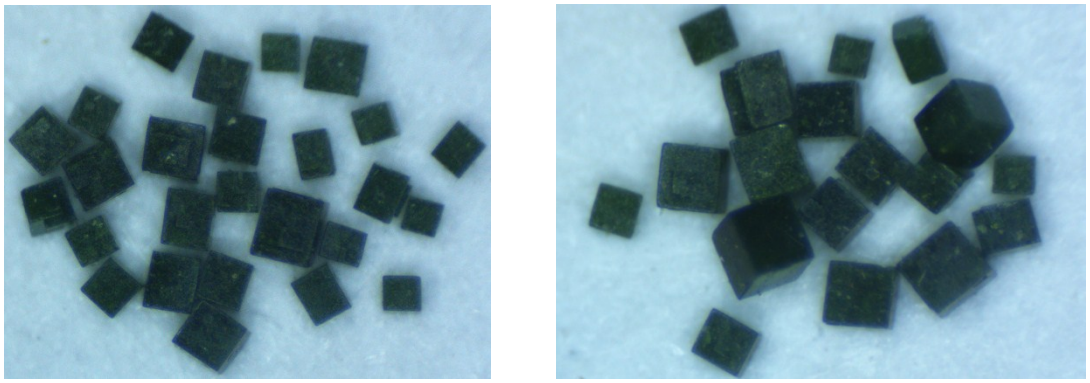

Figure S1 Green cubic crystals of **1-Dy** (left) and **1-Tb** (right).

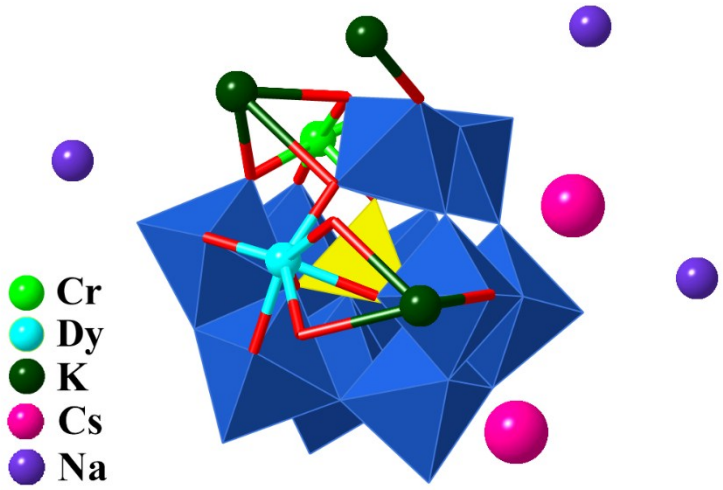

Figure S2 View of the asymmetric unit of **1-Dy**, all lattice water molecules are omited for clarity.

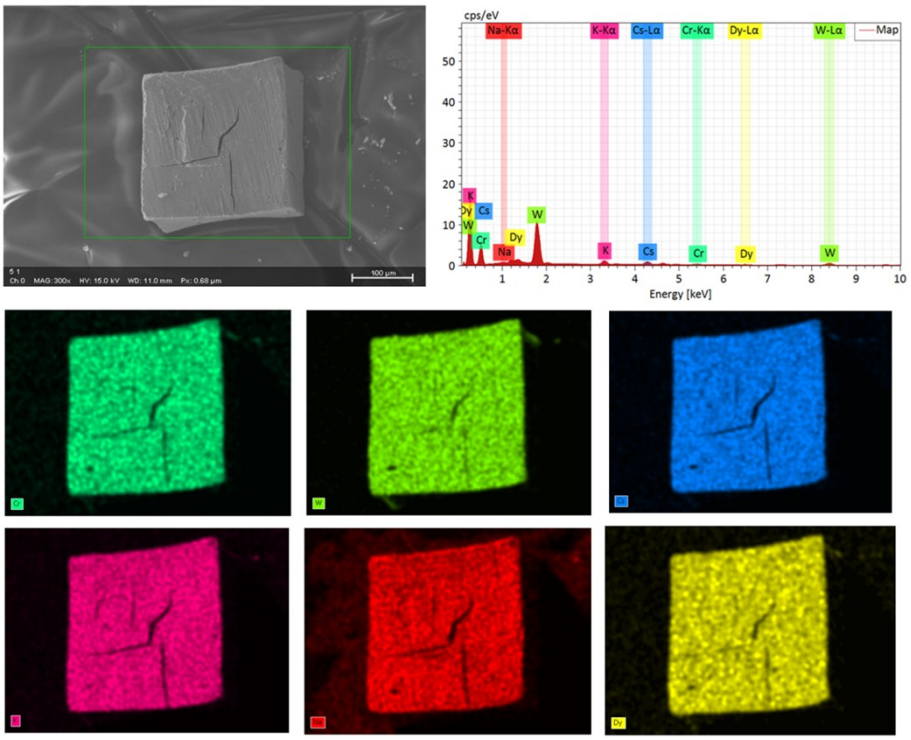

Figure S3 The EDS elemental mappings of **1-Dy**.

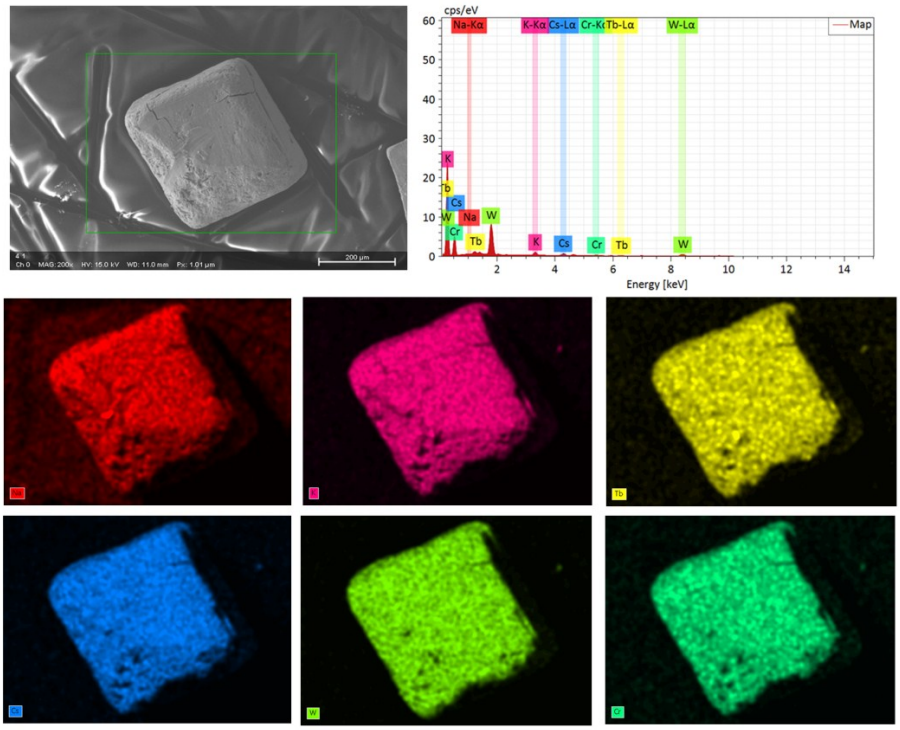

Figure S4 The EDS elemental mappings of Cr, Tb, W for **1-Tb**.

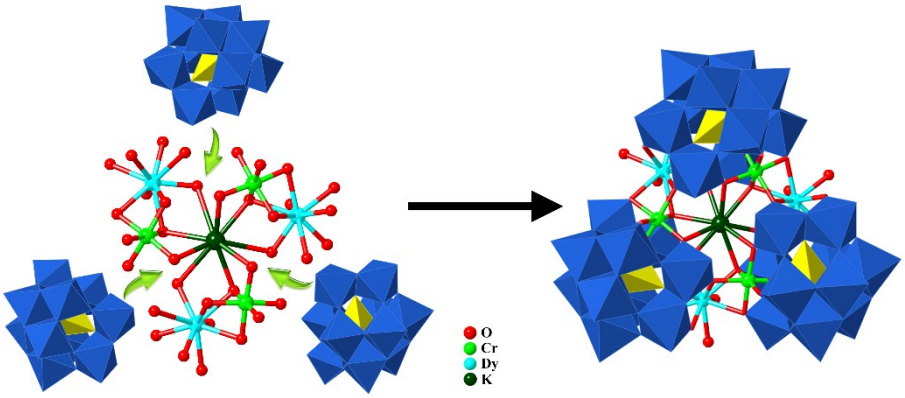

Figure S5 View of the trimeric structure based on seven-nuclearity 3p-3d-4f cluster and dilacunary $[\alpha\text{-}GeW_{10}O_{38}]^{12-}$ fragments.

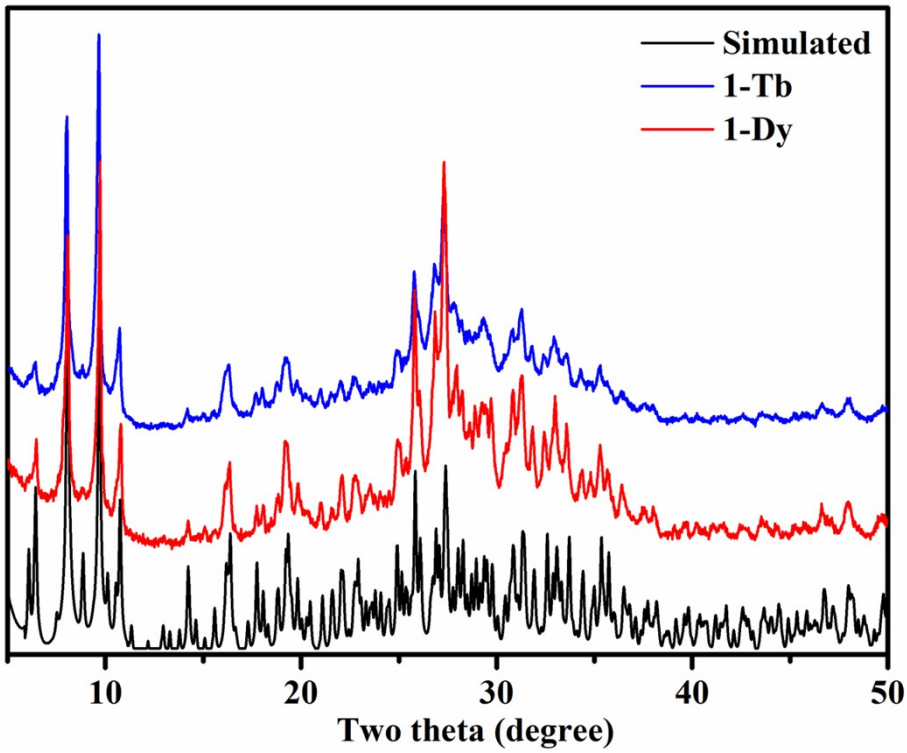

Figure S6 Simulated and experimental PXRD patterns of **1-Dy** and **1-Tb**.

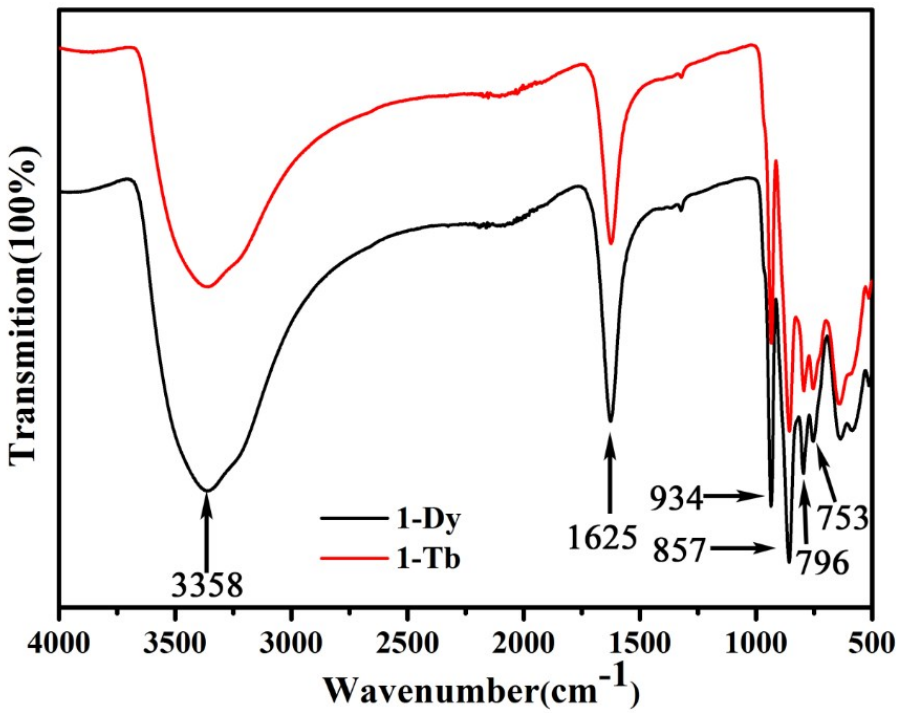

Figure S7 The IR spectra for **1-Dy** and **1-Tb**.

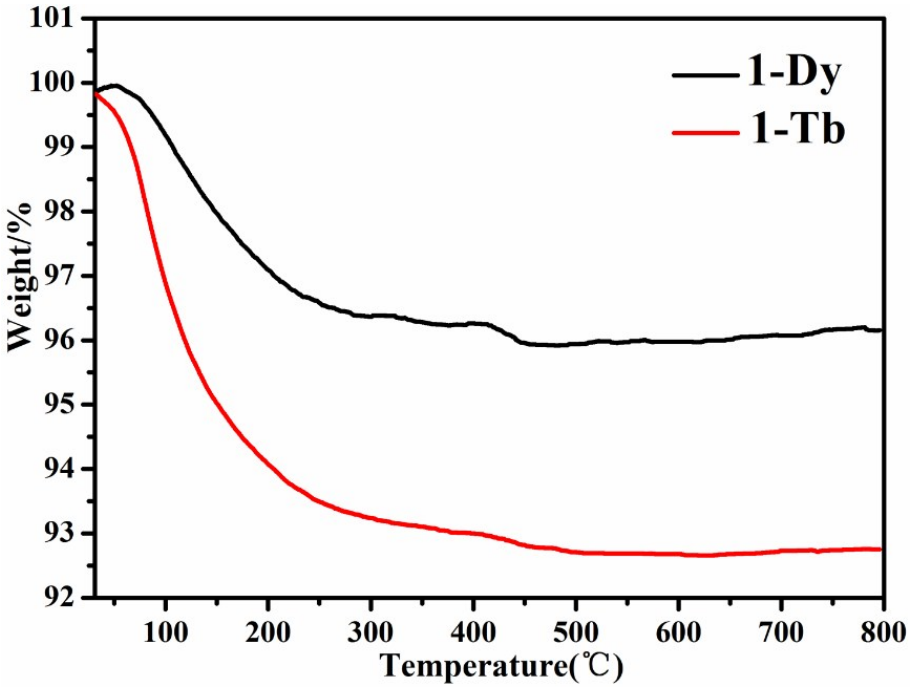

Figure S8 The TG curves of **1-Dy** and **1-Tb**.

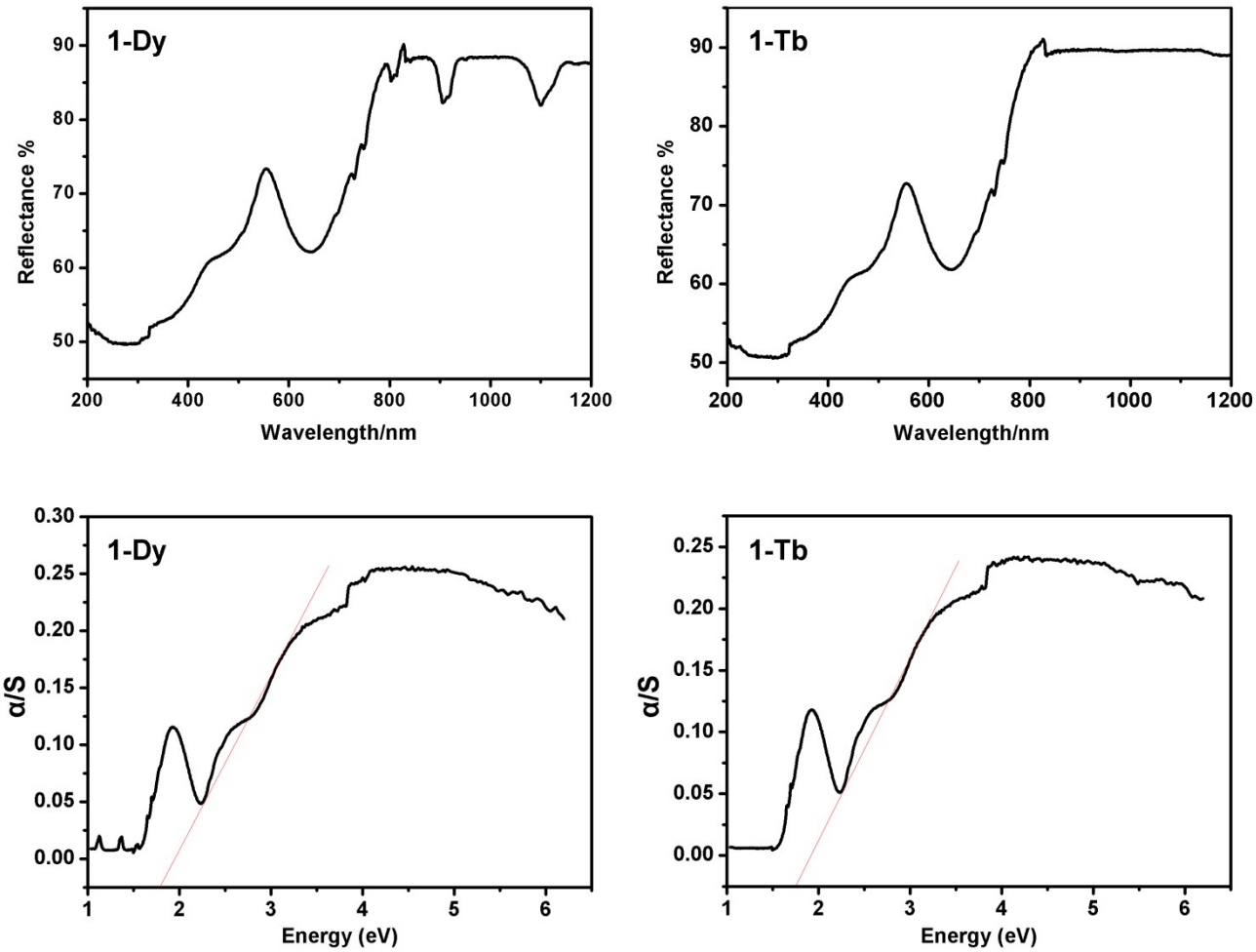

Figure S9 UV - vis absorption spectra of **1-Dy** (a), **1-Tb** (b). The diffuse reflectance UV - vis - NIR spectra of Kubelka - Munk Function *vs.* energy (eV) of **1-Dy** (c), **1-Tb** (d).