Supplementary Information

Title: Crystal Structure, Optical Properties and Thermal Properties of $M_2[W_2O_3(SO_4)_6]$ (M = Y, Eu, Tb, Lu, Bi)

Author(s): V. Wessels[a], S. Kügle[a], H. A. Höppe[a]

[a] Institut für Physik, Universität Augsburg, Universitätsstraße 1, 86159 Augsburg, Germany

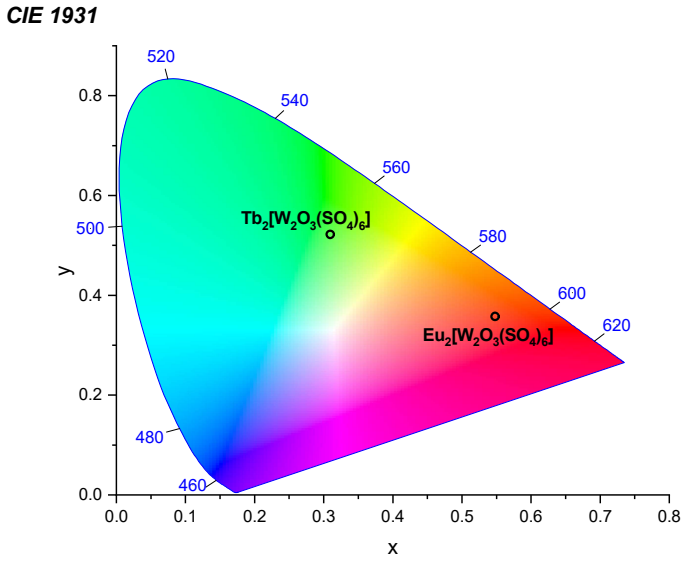

Figure S1 CIE diagram for $Tb_2[W_2O_3(SO_4)_6]$ and $Eu_2[W_2O_3(SO_4)_6]$.

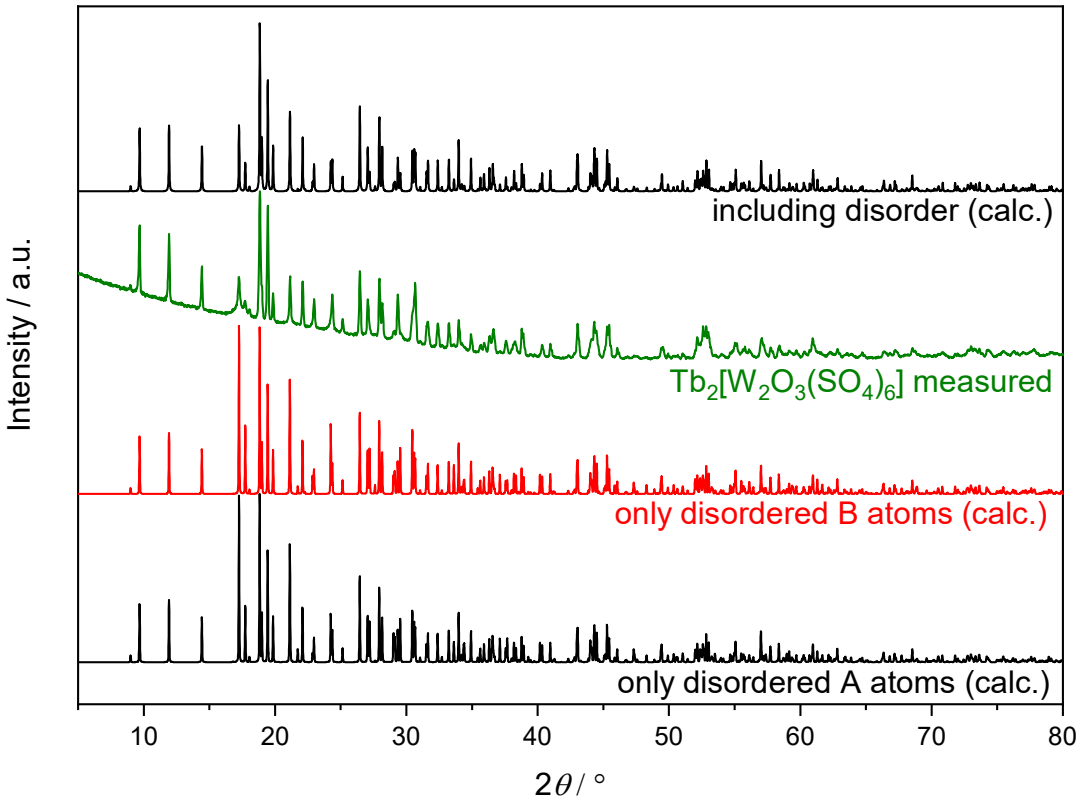

Figure S2 PXRD comparing the measured pattern of $Tb_2[W_2O_3(SO_4)_6]$ with the calculated pattern including the disorder and considering only W1A, O1A, O2A or W1B, O1B, O2B, respectively.

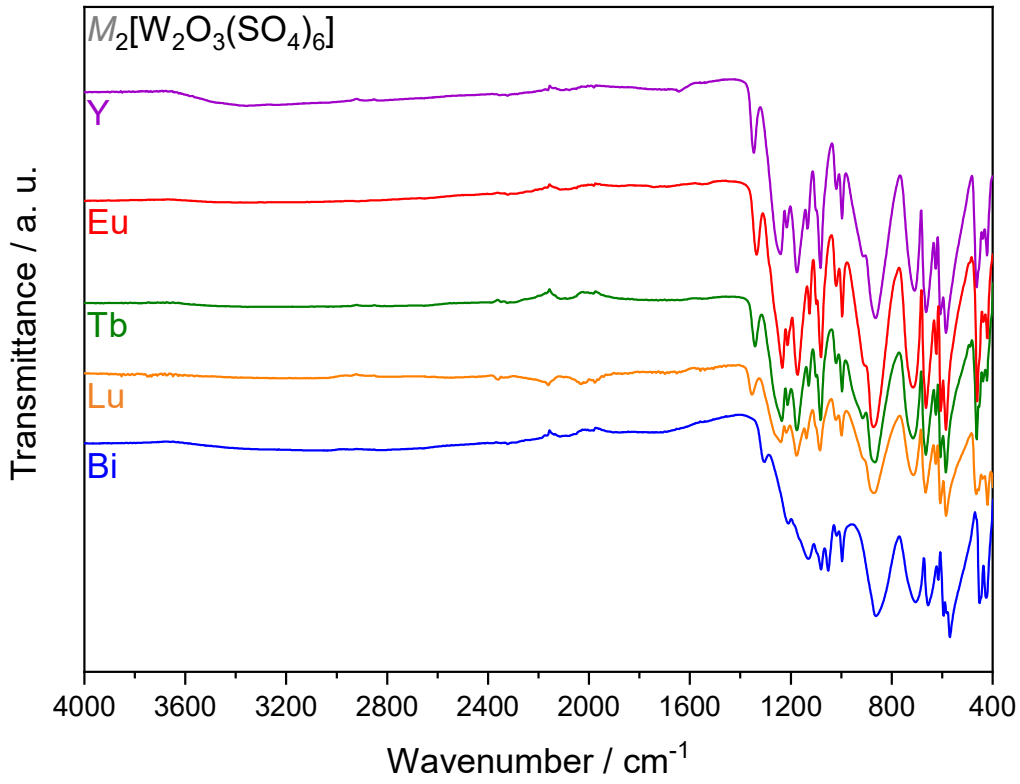

Figure S3 FT-IR spectrum of $M_2[W_2O_3(SO_4)_6]$.

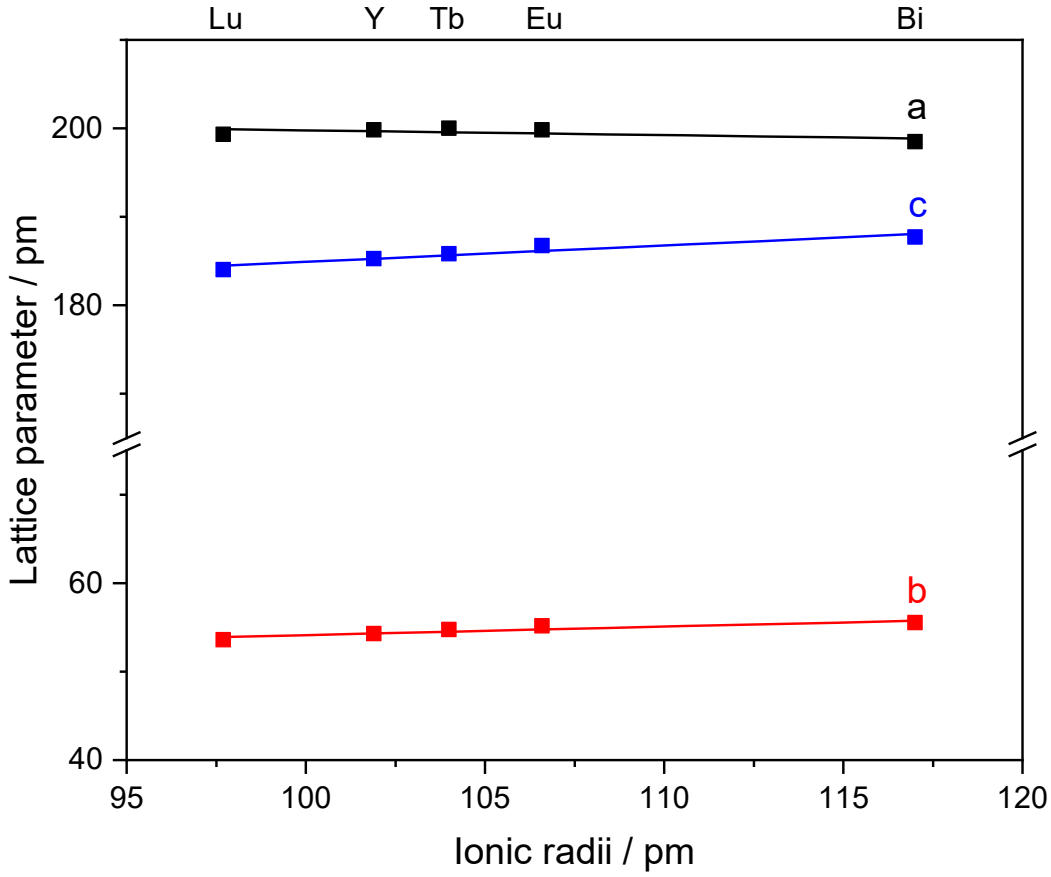

Figure S4 Correlation of the ionic radii of the cations with the lattice parameters *a*, *b,* and *c* of the title compounds.

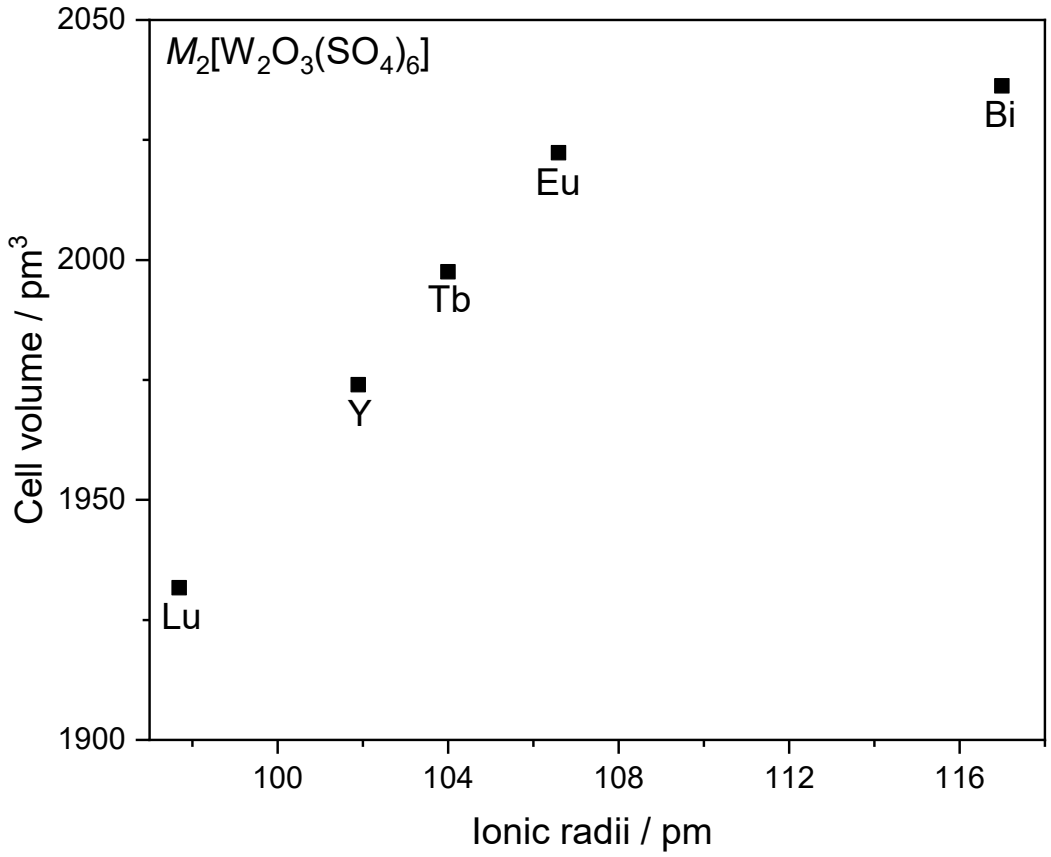

Figure S5 Correlation of the ionic radii with the cell volume of the title compounds.

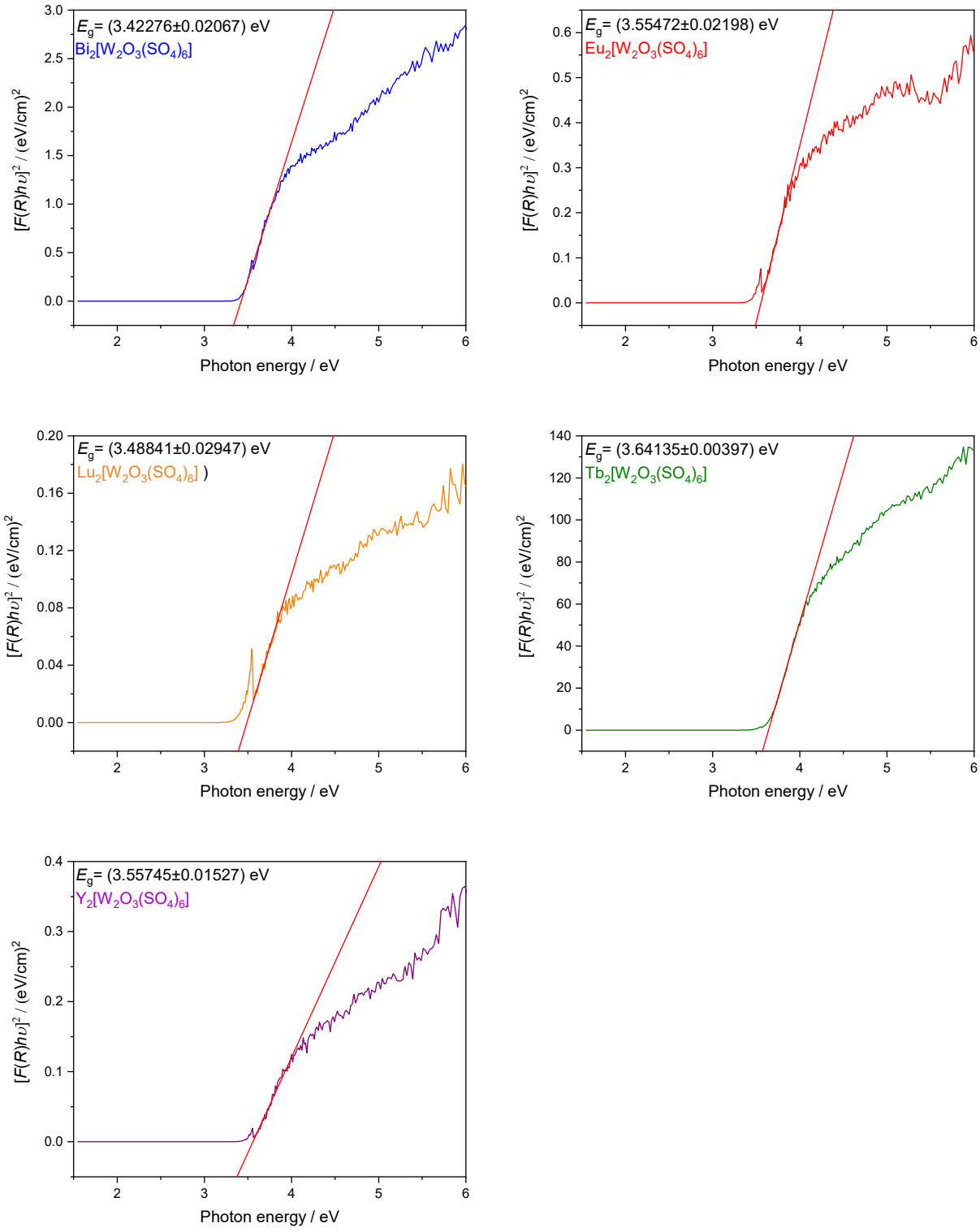

Figure S6 Tauc-plots for the determination of the band gaps of $M_2[W_2O_3(SO_4)_6]$.

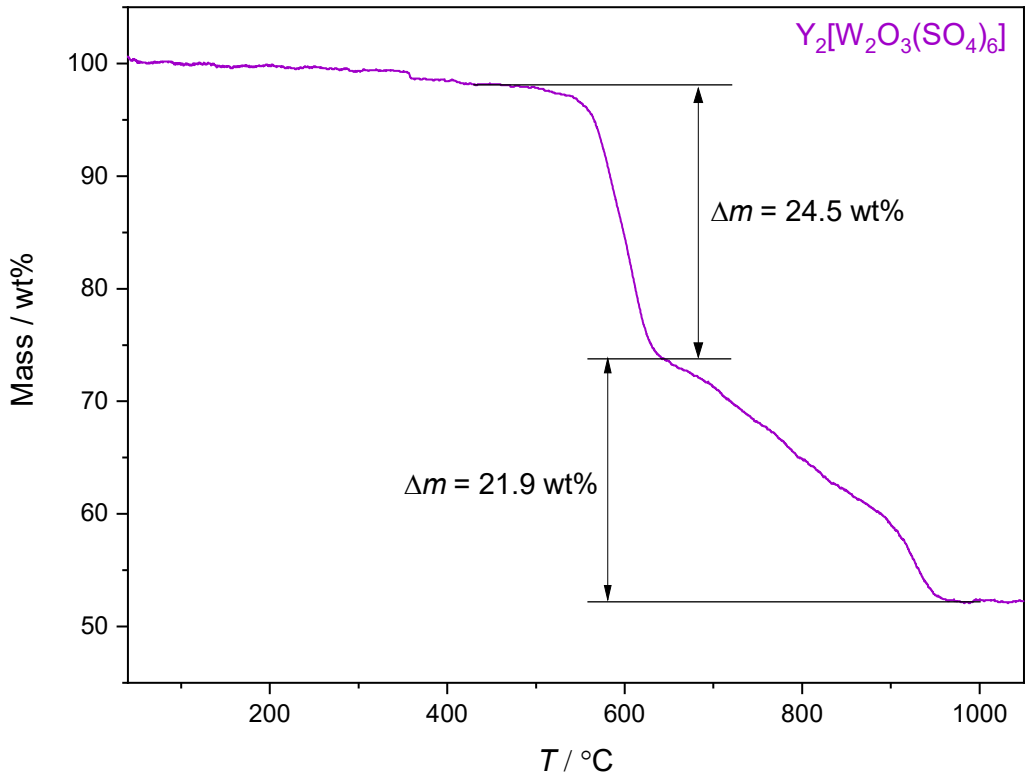

Figure S7 Thermogram of $Y_2[W_2O_3(SO_4)_6]$ recorded up to 1050°C in nitrogen atmosphere.

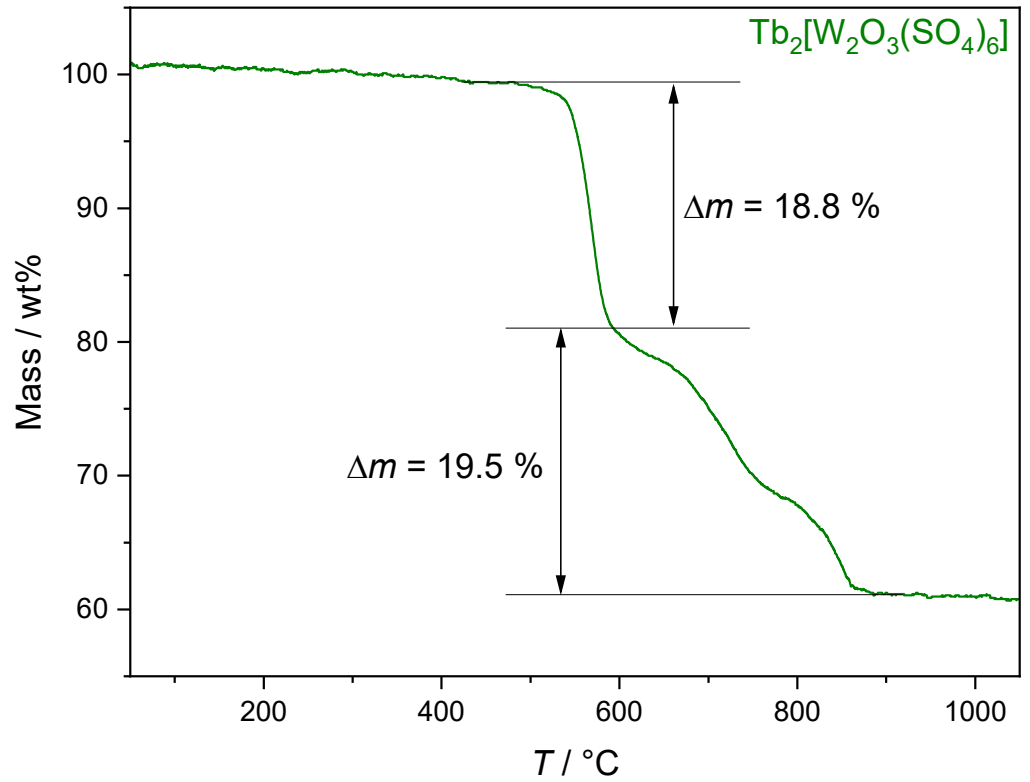

Figure S8 Thermogram of $Tb_2[W_2O_3(SO_4)_6]$ recorded up to 1050°C in nitrogen atmosphere.

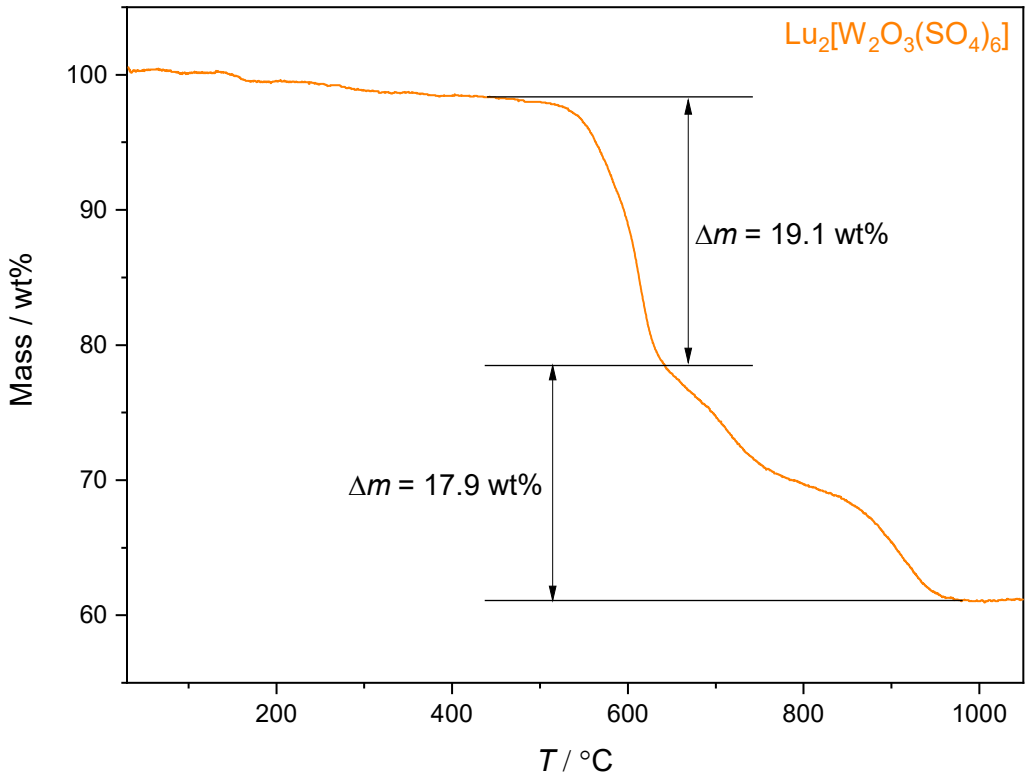

Figure S9 Thermogram of $Lu_2[W_2O_3(SO_4)_6]$ recorded up to 1050°C in nitrogen atmosphere.

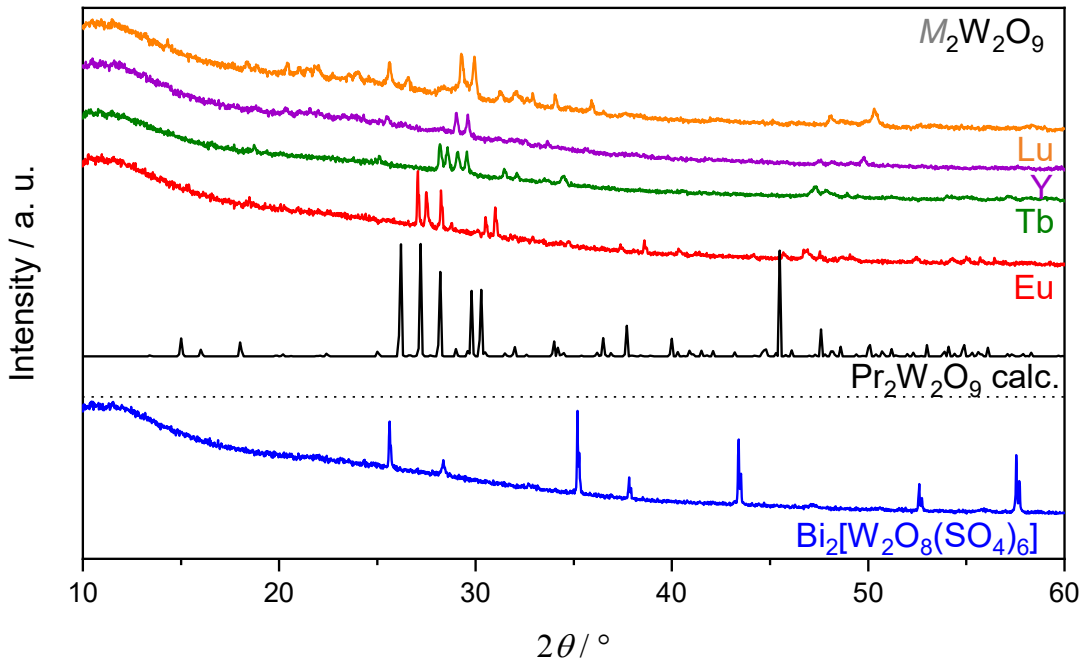

Figure S10 PXRD after thermal treatment by measuring TGA up to 1050°C.

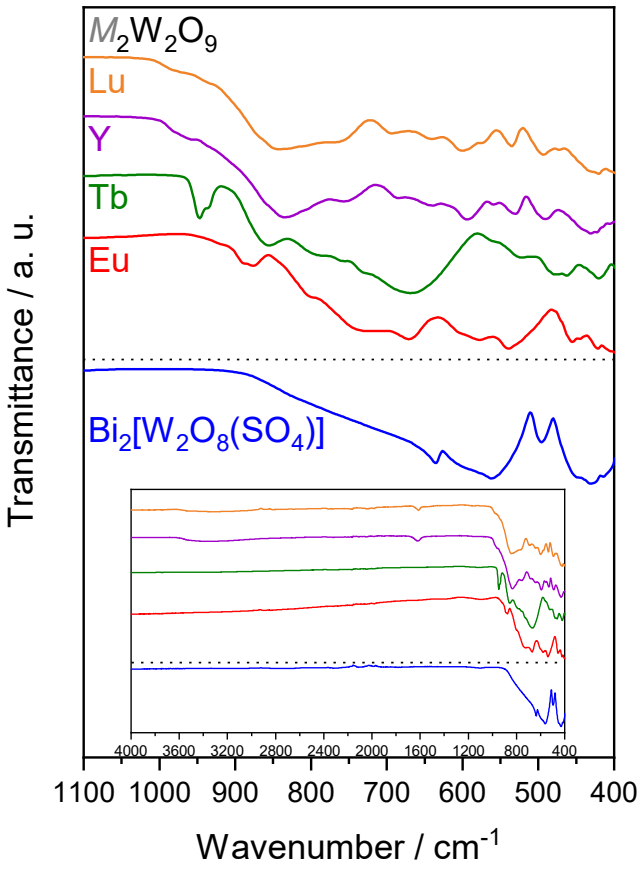

Figure S11 FT-IR spectrum after thermal treatment by measuring TGA up to 1050°C.

Table S1. Atomic coordinates, Wyckoff symbols and isotropic displacement parameters U_{eq} / Å^2 in $Bi_2[W_2O_3(SO_4)_6]$. Standard deviations are given in parentheses.

Atom	Wyckoff symbol	*x*	*y*	*z*	U_{eq}
Bi1	8f	0.18682(2)	0.51513(2)	0.60717(2)	0.00714(4)
W1A	8f	0.44170(2)	0.26236(2)	0.66360(2)	0.00425(3)
O1A	4e	1/2	0.1674(7)	3/4	0.0061(6)
O2A	8f	0.47020(18)	0.0749(6)	0.60497(17)	0.0151(6)
W1B	8f	0.44064(12)	0.7484(4)	0.66337(13)	0.0264(5)
O1B	4e	1/2	0.854(6)	3/4	0.0061(6)
O2B	8f	0.4688(17)	-0.070(6)	0.6000(16)	0.0151(6)
S1	8f	0.29369(4)	0.01048(14)	0.68362(4)	0.00589(12)
O11	8f	0.28155(17)	0.0119(6)	0.75668(15)	0.0153(5)
O12	8f	0.26003(16)	0.2075(6)	0.63948(17)	0.0169(6)
O13	8f	0.27755(16)	-0.2161(5)	0.64617(17)	0.0156(5)
O14	8f	0.37035(15)	0.0465(6)	0.68469(19)	0.0175(6)
S2	8f	0.33797(4)	0.49146(14)	0.52059(4)	0.00549(12)
O21	8f	0.36156(15)	0.7207(5)	0.49682(16)	0.0129(5)
O22	8f	0.26531(13)	0.4930(5)	0.52372(14)	0.0088(4)
O23	8f	0.35834(14)	0.2864(5)	0.48043(16)	0.0131(5)
O24	8f	0.37655(14)	0.4575(5)	0.59943(14)	0.0109(4)
S3	8f	0.58483(4)	0.54058(17)	0.68159(4)	0.008827(13)

O31	8f	0.61717(18)	0.3512(7)	0.64826(19)	0.0220(7)
O32	8f	0.60307(15)	0.7824(6)	0.66168(17)	0.0157(5)
O33	8f	0.59643(15)	0.5158(5)	0.76103(15)	0.0134(5)
O34	8f	0.50685(14)	0.5227(5)	0.65645(16)	0.0130(5)

Table S2. Anisotropic displacement parameters U_{ij} / Å^2 in $Bi_2[W_2O_3(SO_4)_6]$. Standard deviations are given in parentheses.

Atom	*U*11	*U*22	*U*33	*U*12	*U*13	*U*23
Bi1	0.00661(5)	0.00689(5)	0.00770(5)	0.00029(4)	0.00063(3)	0.00011(4)
W1A	0.00329(5)	0.00546(6)	0.00352(5)	-0.00033(4)	-0.00067(4)	-0.00004(4)
O1A	0.0034(13)	0.0061(14)	0.0077(14)	0.0000(0)	-0.0018(11)	0.0000(0)
O2A	0.0192(15)	0.0152(13)	0.0101(12)	0.0051(12)	0.0006(11)	-0.0048(11)
W1B	0.0271(10)	0.0170(9)	0.0324(11)	0.0018(7)	-0.0023(8)	-0.0007(7)
O1B	0.0034(13)	0.0061(14)	0.0077(14)	0.0000(0)	-0.0018(11)	0.0000(0)
O2B	0.0192(15)	0.0152(13)	0.0101(12)	0.0051(12)	0.0006(11)	-0.0048(11)
S1	0.0062(3)	0.0054(3)	0.0056(3)	-0.0003(2)	0.0000(2)	-0.0001(2)
O11	0.0235(14)	0.0173(13)	0.0052(10)	0.0003(11)	0.0029(10)	0.0002(9)
O12	0.0175(13)	0.0180(13)	0.0162(12)	0.0100(11)	0.0054(10)	0.0094(11)
O13	0.0170(13)	0.0122(12)	0.0189(13)	-0.0074(10)	0.0065(10)	-0.0088(10)
O14	0.0062(11)	0.0192(14)	0.0259(15)	-0.0014(10)	-0.0007(10)	0.0092(12)
S2	0.0058(3)	0.0054(3)	0.0051(3)	-0.0001(2)	0.0004(2)	0.0003(2)
O21	0.0128(11)	0.0106(11)	0.0151(11)	-0.0015(9)	0.0016(9)	0.0058(9)
O22	0.0069(10)	0.0123(11)	0.0068(9)	0.0006(8)	0.0006(7)	0.0002(8)
O23	0.0105(11)	0.0143(12)	0.0149(12)	0.0001(9)	0.0032(9)	-0.0083(10)
O24	0.0084(10)	0.0183(12)	0.0052(9)	0.0017(9)	-0.0010(8)	0.0018(9)
S3	0.0056(3)	0.0132(3)	0.0062(3)	0.0000(3)	0.0017(2)	0.0010(3)
O31	0.0228(15)	0.0216(15)	0.0237(15)	0.0091(13)	0.0097(13)	-0.0030(13)
O32	0.0133(12)	0.0176(13)	0.0165(12)	-0.007(1)	0.0035(10)	0.0041(10)
O33	0.0135(12)	0.0195(13)	0.0066(10)	-0.0086(10)	0.0001(8)	0.0026(9)
O34	0.0071(10)	0.0173(13)	0.0135(11)	-0.0029(9)	-0.0016(9)	0.0043(10)

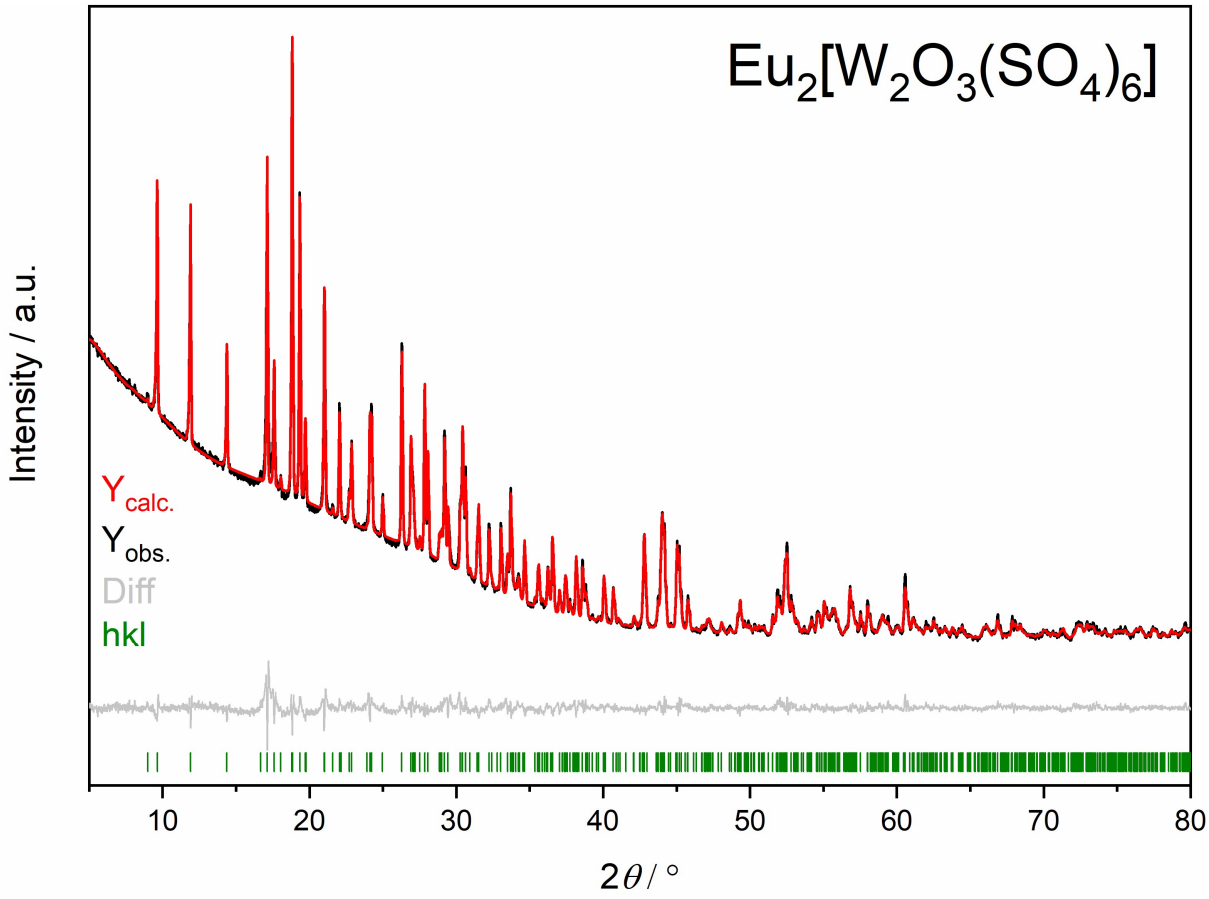

Figure S12 Rietveld refinement of $Eu_2[W_2O_3(SO_4)_6]$.

Table S3 Crystal data and structure refinement of $Eu_2[W_2O_3(SO_4)_6]$ determined from powered XRD data via Rietveld refinement. Respective standard deviations are given in parentheses.

M /g mol^{-1}	1295.98
temperature / K	300(2)
space group	*C*2/*c* (no. 15)
a / Å	20.0032(5)
b / Å	5.51969(13)
c / Å	18.6673(4)
β /°	100.7616(17)
V / Å^3	2024.84(8)
Z	4
ρ / g·cm^{-3}	4.32
radiation; wavelength λ / Å	Cu-K_α; 1.54184
diffractometer	Bruker D8 Advance
θ range / °	2.5-40
R_{Bragg}	0.011
R_p	0.017
R_{wp}	0.024
GooF	2.30
site occupation scenario A	0.8841(1)

Table S4 Polyhedron deviation / % of tungstate octahedra ordered by central atoms W1A and W1B.

Compound	W1A	W1B
$Lu_2[W_2O_3(SO_4)_6]$	-8.04	-20.46
$Y_2[W_2O_3(SO_4)_6]$	-5.13	-26.53
$Tb_2[W_2O_3(SO_4)_6]$	-5.91	-24.93
$Eu_2[W_2O_3(SO_4)_6]$	-5.06	-10.31
$Bi_2[W_2O_3(SO_4)_6]$	-4.47	-15.16