*R*CuMg$_2$ compounds (*R* = Dy–Tm, Lu): crystal structure, chemical bonding and magnetic properties

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Supplementary materials

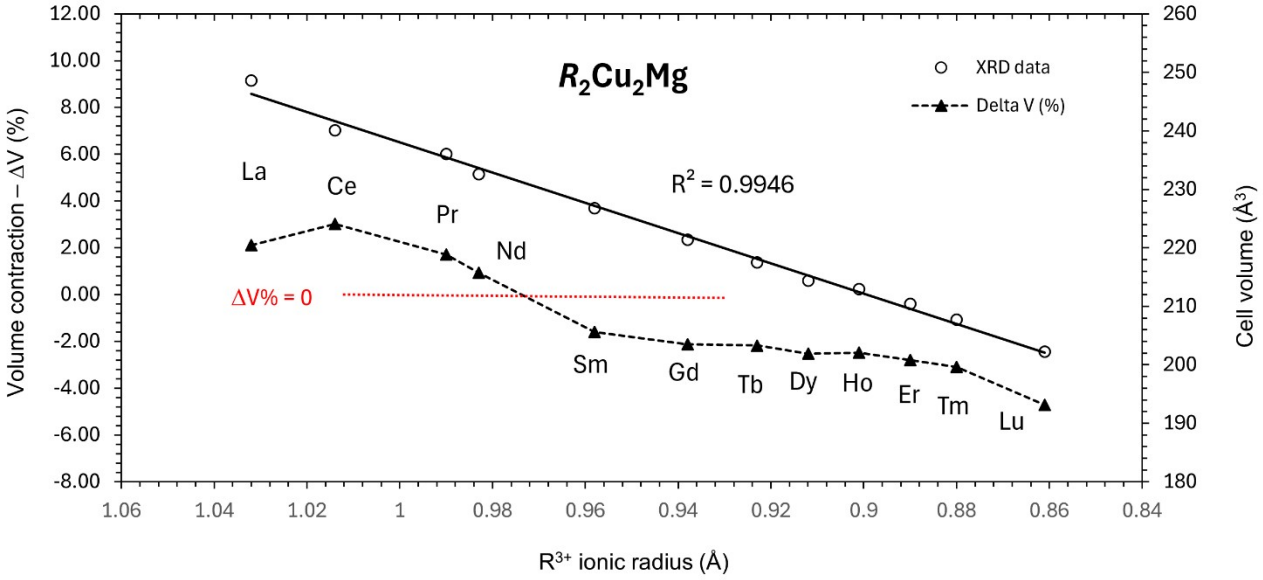

Figure S1. Unit cell volume and volume contraction trends for R_2Cu_2Mg compounds.

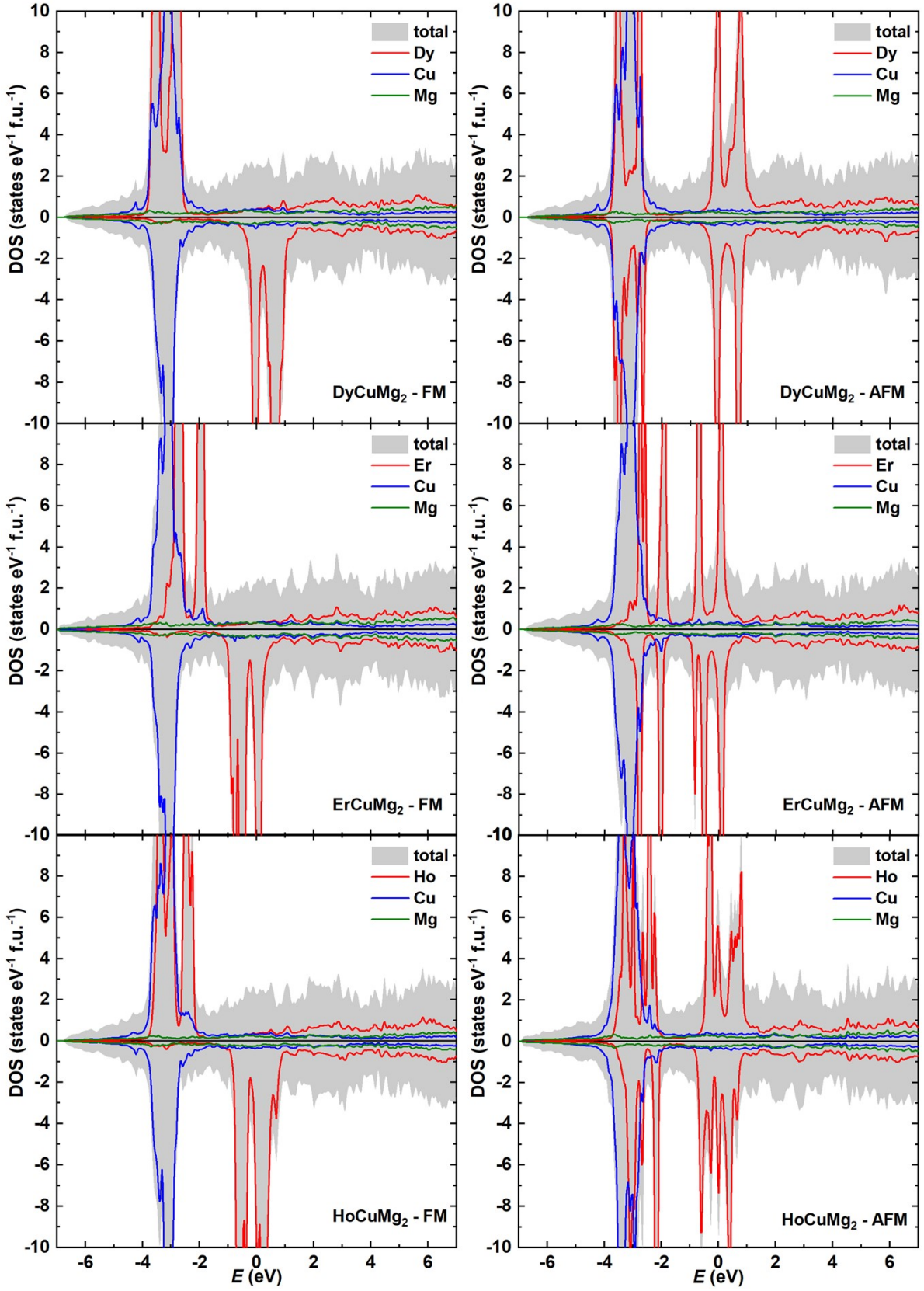

Fig. S2. Total and atomic resolved electronic density of states calculated for {Dy, Er, Ho}$CuMg_2$ assuming ferromagnetic (FM) and antiferromagnetic (AFM) spin alignments in their magnetic structures.

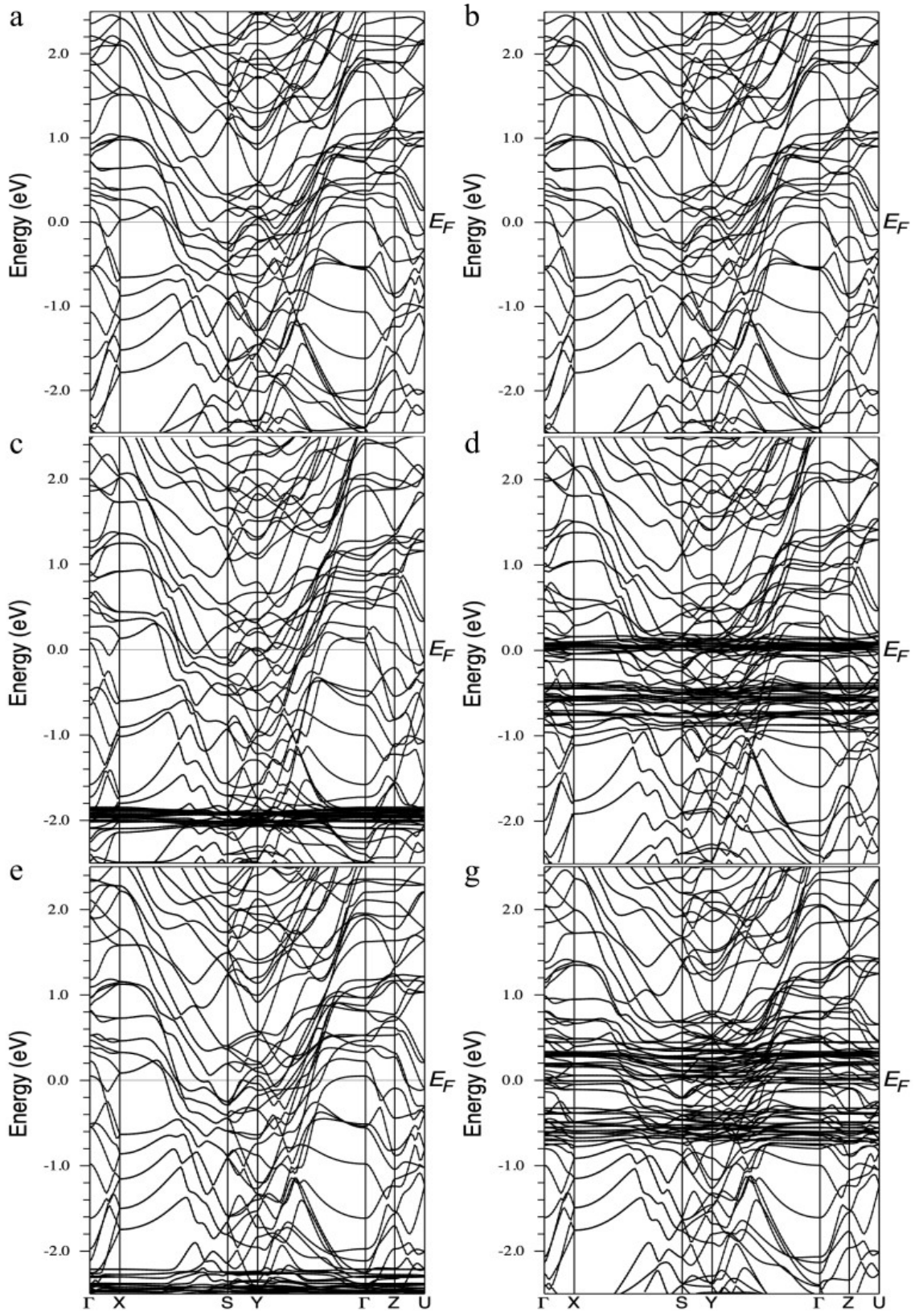

Fig. S3. Electronic band structures for ferromagnetic DyCuMg2 (a, b), $ErCuMg_2$ (c, d), $HoCuMg_2$ (e, g). In the panels a, c, e are presented spin up bands, whereas in b, d, g - spin down.

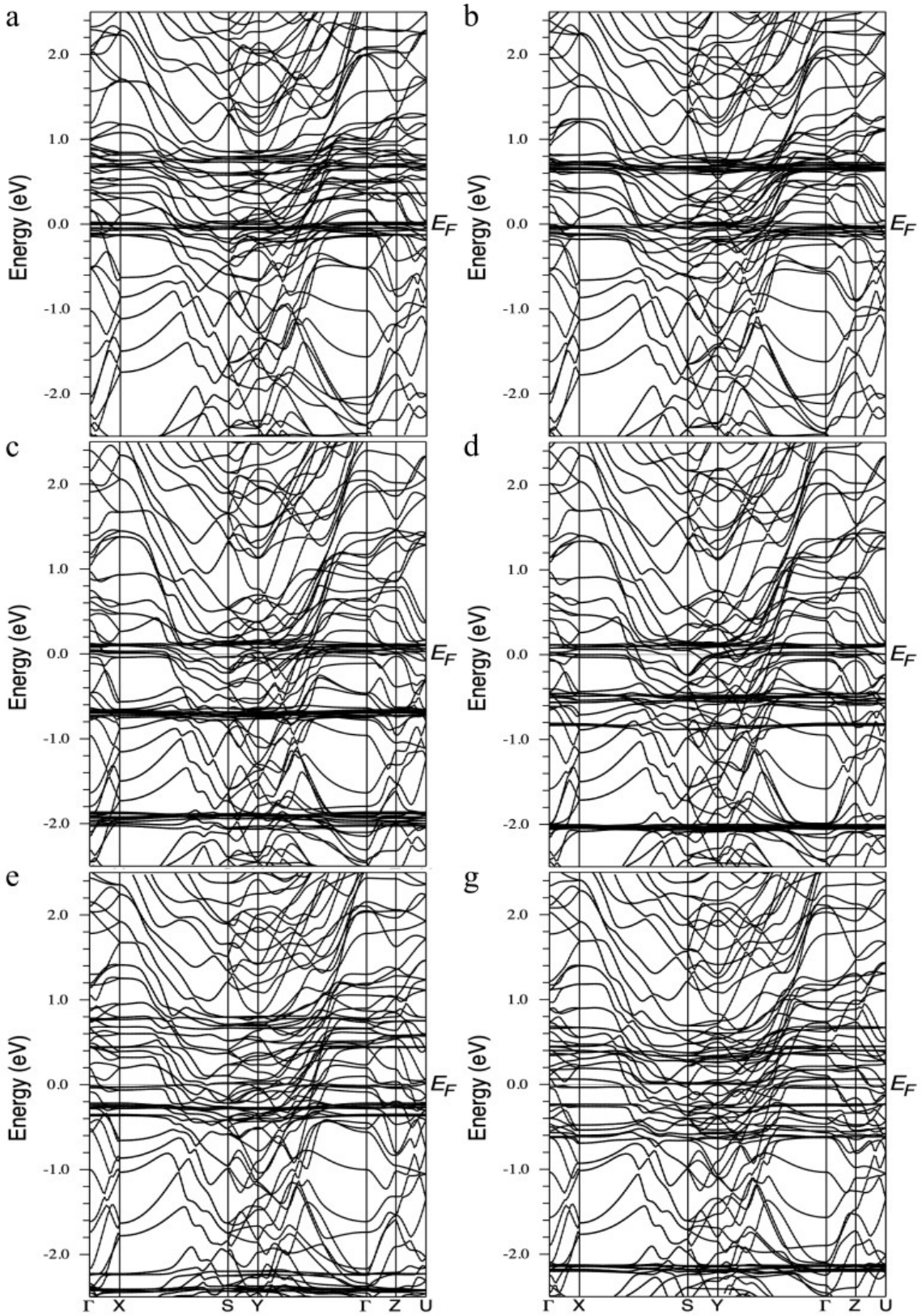

Fig. S4. Electronic band structures for antiferromagnetic DyCuMg2 (a, b), $ErCuMg_2$ (c, d), $HoCuMg_2$ (e, g). In the panels a, c, e are presented spin up bands, whereas in b, d, g - spin down.

Table S1. Refined (from XRPD data) and optimized (DFT) atomic coordinates for the studied $RCuMg_2$ compounds.

Atom	Site	Refined atomic coordinates			Optimized atomic coordinates		
		x/a	*y/b*	*z/c*	*x/a*	*y/b*	*z/c*
$DyCuMg_2$							
Dy1	4*j*	0.0478(2)	½	0.3817(5)	0.048280	½	0.376310
Dy2	2*f*	¼	½	0.1780(4)	¼	½	0.184960
Dy3	2*f*	¼	½	0.5752(4)	¼	½	0.576100
Cu1	4*i*	0.0926(9)	0	0.5264(7)	0.090700	0	0.532990
Cu2	4*i*	0.1015(10)	0	0.2048(8)	0.091780	0	0.219550
Mg1	4*j*	0.4977(13)	½	0.122(3)	0.508610	½	0.123760
Mg2	2*e*	¼	0	0.392(3)	¼	0	0.378660
Mg3	4*i*	0.624(3)	0	0.287(2)	0.622740	0	0.262660
Mg4	4*i*	0.122(3)	0	-0.012(3)	0.133760	0	0.014870
Mg5	2*f*	¼	½	0.860(3)	¼	½	0.869360
Atom	**Site**	**Refined atomic coordinates**			**Optimized atomic coordinates**		
		x/a	*y/b*	*z/c*	*x/a*	*y/b*	*z/c*
$HoCuMg_2$							
Ho1	4*j*	0.0431(3)	½	0.3787(8)	0.050600	½	0.376670
Ho2	2*f*	¼	½	0.1832(5)	¼	½	0.184680
Ho3	2*f*	¼	½	0.5752(5)	¼	½	0.573180
Cu1	4*i*	0.1017(8)	0	0.5323(8)	0.090210	0	0.533530
Cu2	4*i*	0.0887(8)	0	0.2201(9)	0.090410	0	0.219320
Mg1	4*j*	0.5324(14)	½	0.137(4)	0.509980	½	0.123220
Mg2	2*e*	¼	0	0.378(3)	¼	0	0.377520
Mg3	4*i*	0.6456(19)	0	0.267(2)	0.622250	0	0.264440
Mg4	4*i*	0.117(2)	0	0.004(3)	0.133980	0	0.014980
Mg5	2*f*	¼	½	0.856(3)	¼	½	0.867420
Atom	**Site**	**Refined atomic coordinates**			**Optimized atomic coordinates**		
		x/a	*y/b*	*z/c*	*x/a*	*y/b*	*z/c*
$ErCuMg_2$							
Er1	4*j*	0.0465(4)	½	0.3807(9)	0.05132	½	0.37712
Er2	2*f*	¼	½	0.1840(6)	¼	½	0.18456
Er3	2*f*	¼	½	0.5739(7)	¼	½	0.57251
Cu1	4*i*	0.1010(11)	0	0.5325(12)	0.08983	0	0.53376
Cu2	4*i*	0.0839(12)	0	0.2266(12)	0.09125	0	0.21929
Mg1	4*j*	0.530(2)	½	0.133(5)	0.509480	½	0.123050
Mg2	2*e*	¼	0	0.375(5)	¼	0	0.376440
Mg3	4*i*	0.643(3)	0	0.270(4)	0.621840	0	0.264310
Mg4	4*i*	0.118(3)	0	0.003(4)	0.133880	0	0.014240
Mg5	2*f*	¼	½	0.853(4)	¼	½	0.86759

Atom	Site	Refined atomic coordinates			Atom	Site	Optimized atomic coordinates		
		x/a	***y/b***	***z/c***			***x/a***	***y/b***	***z/c***
Tm1	4*j*	0.0451(3)	½	0.3821(7)	Lu1	4*j*	0.04742	½	0.37804
Tm2	2*f*	¼	½	0.1852(5)	Lu2	2*f*	¼	½	0.18520
Tm3	2*f*	¼	½	0.5743(5)	Lu3	2*f*	¼	½	0.57546
Cu1	4*i*	0.0983(10)	0	0.5335(10)	Cu1	4*i*	0.09265	0	0.53275
Cu2	4*i*	0.086(1)	0	0.2263(11)	Cu2	4*i*	0.09335	0	0.22338
Mg1	4*j*	0.5207(16)	½	0.134(4)	Mg1	4*j*	0.51005	½	0.12383
Mg2	2*e*	¼	0	0.380(4)	Mg2	2*e*	¼	0	0.37930
Mg3	4*i*	0.622(3)	0	0.269(3)	Mg3	4*i*	0.62436	0	0.26482
Mg4	4*i*	0.110(3)	0	-0.002(3)	Mg4	4*i*	0.13458	0	0.01572
Mg5	2*f*	¼	½	0.838(3)	Mg5	2*f*	¼	½	0.86903