

# Ternary Thallides $RE\text{MgTl}$ ( $RE = \text{Y, La} - \text{Nd, Sm, Gd} - \text{Tm, Lu}$ )

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The rare earth metal ( $RE$ )–magnesium–thallides  $RE\text{MgTl}$  ( $RE = \text{Y, La} - \text{Nd, Sm, Gd} - \text{Tm, Lu}$ ) were prepared from the elements in sealed tantalum tubes in a water-cooled sample chamber of a high-frequency furnace. The thallides were characterized through their X-ray powder patterns. They crystallize with the hexagonal  $\text{ZrNiAl}$  type structure, space group  $P6_2m$ , with three formula units per cell. Four structures were refined from X-ray single crystal diffractometer data:  $a = 750.5(1)$ ,  $c = 459.85(8)$  pm,  $wR2 = 0.0491$ , 364  $F^2$  values, 14 variables for  $\text{YMgTl}$ ;  $a = 781.3(1)$ ,  $c = 477.84(8)$  pm,  $wR2 = 0.0640$ ,  $\text{BASF} = 0.09(2)$ , 425  $F^2$  values, 15 variables for  $\text{LaMgTl}$ ;  $a = 774.1(1)$ ,  $c = 473.75(7)$  pm,  $wR2 = 0.0405$ , 295  $F^2$  values, 14 variables for  $\text{CeMgTl}$ ;  $a = 760.3(1)$ ,  $c = 465.93(8)$  pm,  $wR2 = 0.0262$ , 287  $F^2$  values, 14 variables for  $\text{SmMgTl}$ . The  $\text{PrMgTl}$ ,  $\text{NdMgTl}$ ,  $\text{GdMgTl}$ ,  $\text{TbMgTl}$ , and  $\text{DyMgTl}$  structures have been analyzed using the Rietveld technique. The  $RE\text{MgTl}$  structures contain two crystallographically independent thallium sites, both with tri-capped trigonal prismatic coordination:  $\text{Tl1Mg}_3RE_6$  and  $\text{Tl2Mg}_6RE_3$ . Together the magnesium and thallium atoms form three-dimensional  $[\text{MgTl}]$  networks with  $\text{Mg} - \text{Mg}$  distances of 327 and  $\text{Mg} - \text{Tl}$  distances in the range 299 – 303 pm (data for  $\text{CeMgTl}$ ).

*Key words:* Rare Earth Compounds, Thallides, Crystal Chemistry