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## Modelling the thermodynamic properties of $\text{TiCl}_3$ medium

The reduction of titanium tetrachloride ( $\text{TiCl}_4$ ) with magnesium (Mg) results in the production of intermediates such as titanium trichloride ( $\text{TiCl}_3$ ) and titanium dichloride ( $\text{TiCl}_2$ ). Experimental work has been done to develop a continuous reduction process using  $\text{TiCl}_3$  and  $\text{TiCl}_2$ . However, more investigations still need to be done to understand these mediums and their interactions. In this study, we will be looking at two  $\text{TiCl}_3$  polymorphs as a potential medium for titanium production. We employ the DL\_POLY code to understand the effect of temperature on the  $\text{TiCl}_3$  mediums with R-3 and P3112 space groups. It was noted from the Gibbs free energy that reactions in the R-3 medium are not favourable at 50 K – 2000 K. The results of this study give us more insight into the  $\text{TiCl}_3$  medium as a potential medium for evaluating titanium.

### Apply for student award at which level:

PhD

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Yes, I ACCEPT

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