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## Effect of temperature on $\beta$ -TiCl<sub>3</sub> medium

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The magnesiothermic reduction of titanium tetrachloride (TiCl<sub>4</sub>) results in the formation of titanium subchlorides such as titanium trichloride (TiCl<sub>3</sub>) and titanium dichloride (TiCl<sub>2</sub>). However, this process occurs extremely fast and it is not suitable for the development of a continuous reduction process. In this study, classical molecular dynamic calculations were performed to understand the influence of temperature on the TiCl<sub>3</sub> ( $\beta$ -TiCl<sub>3</sub>) structure (using rigid ion and shell model) with P63/mcm space group, employing the DL\_POLY code. It was found that for the rigid ion model chlorine diffuses at 300 K. The entropy and Gibbs free energy was used to deduce the behaviour of atoms and the spontaneity of the structure. Positive entropy is noted at 600 K – 700 K for the rigid ion model and at 700 K for the shell model, indicating possible melting. In addition, the system was also observed to be spontaneous (favourable) for both models at 50 K – 2000 K. The results of this study give us more insight into the TiCl<sub>3</sub> medium as a potential medium for evaluating titanium.

**Apply to be considered for a student ; award (Yes / No)?**

Yes

**Level for award;(Hons, MSc, PhD, N/A)?**

PhD

**Primary authors:** Ms MAZIBUKO, Andile (University of Limpopo); Prof. CHAUKE, Hasani (University of Limpopo)

**Co-author:** NGOEPE, Phuti (University of Limpopo)

**Presenter:** Ms MAZIBUKO, Andile (University of Limpopo)

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