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Evaluating the small Ti₇ cluster in α -TiCl₃ medium

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The Kroll process is a widely used technique in the commercial production of titanium. This process involves a magnesiothermic reduction of titanium tetrachloride (TiCl₄). Although this process has several advantages, it is, however, not suitable for the development of a continuous reduction process. Recent studies have introduced a magnesiothermic reduction of other transition metal halides such as titanium trichloride (TiCl₃) or titanium dichloride (TiCl₂). This is in an attempt to develop a high-speed (semi-)continuous reduction process. In this study, classical molecular dynamic calculations were performed to understand the influence of temperature on the Ti₇/TiCl₃ (α -TiCl₃) system. The DL_POLY code was used to evaluate the temperature dependence of the structure. It was found that the cluster maintains its pentagonal bipyramid geometry. The entropy and Gibbs free energy were used to deduce the behaviour of atoms and the spontaneity of the structure. It was observed that the entropy graph shows the system to be well arranged (ordered) at the temperature range of 50 K – 2000 K. Furthermore, it was also observed that the system is spontaneous (favourable) at 50 K. The results of this study give us more insight into the TiCl₃ 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

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