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FT-IR CHARACTERIZATION OF TITANIUM TETRABUTOXIDE CATALYST OF ETHYLENE DIMERIZATION: A DFT STUDY

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Ethylene dimerization is a topic of major fundamental and applied importance. It has triggered much research and scientific effort to improve performance of the catalysts used in the industrial scale. Of the metals studied, titanium-based compounds have been found to be ideally suited, giving high yields of 1-butene. Computational chemistry, and in particular density functional theory (DFT), has been proven to give insights for a better understanding of reaction mechanisms that play a role in homogeneous catalysis. Vibrational spectroscopy is an excellent method for structural analysis and the determination of molecular interactions. In this research, the DFT calculations were done to study optimized structure and theoretical FT-IR spectroscopic data for the titanium tetrabutoxide as a conventional catalyst in the ethylene dimerization. In this regard, firstly the B3LYP/LANL2DZ basis set for Ti atom and B3LYP/6-31G basis set for C, H, and O atoms were used. After optimization, configuration of the titanium tetrabutoxide structure was disrupted. Therefore, optimization method was qualified by the B3LYP/6-31+G (d,p) basis set for all atoms. The results revealed a tetrahedral structure in gas phase with basic parameters of $r(\text{Ti}\cdots\text{O})$ 1.81 Å and $\theta(\text{O}-\text{Ti}\cdots\text{O}) \approx 108.39^\circ$. The comparison of theoretical and experimental frequencies of vibrational assignments in the FT-IR spectrum showed that all frequencies computed by the DFT had good agreement with those observed in the experimental results.

Biography

Seyed Hamed Mahdaviyani received his BSc degree in Chemical Engineering from Amirkabir University of Technology, Tehran and his MSc degree in Chemical Engineering from Iran University of Science and Technology, Tehran, Iran. He has many publications including 15 high quality peer-reviewed papers in scientific journals and international conferences, a book chapter, an Iran patent and several research and technical reports. He received several honours and awards for his outstanding efforts in his research works. In December 2015, he was selected as the first person of Superior Industrialist and Distinguished Researcher in the Festival of Research and Technology of Oil Industry in Tehran, Iran. He has been invited to the several reputed international conferences as a keynote speaker. He has received certificate of reviewing from Elsevier in recognition of the review made for *Applied Catalysis A: General* in March 2016.

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