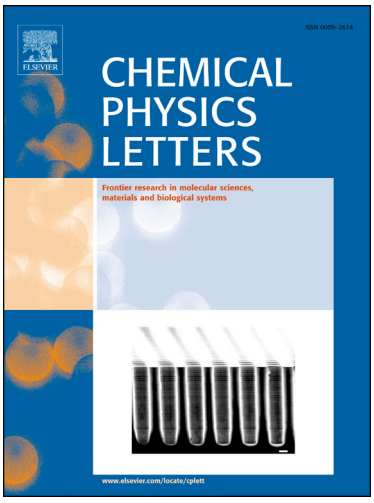

Research paper

Infrared Spectroscopy and Density Functional Calculations on Titanium-Dinitrogen Complexes

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PII: S0009-2614(18)30187-8
DOI: https://doi.org/10.1016/j.cplett.2018.03.009
Reference: CPLETT 35490

To appear in: *Chemical Physics Letters*

Received Date: 1 January 2018
Revised Date: 2 March 2018
Accepted Date: 6 March 2018

Please cite this article as: H-W. Yoo, C. Choi, S. Gyeong Cho, Y. Jung, M. Yong Choi, Infrared Spectroscopy and Density Functional Calculations on Titanium-Dinitrogen Complexes, *Chemical Physics Letters* (2018), doi: https://doi.org/10.1016/j.cplett.2018.03.009

Infrared Spectroscopy and Density Functional Calculations on Titanium-Dinitrogen Complexes

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A B S T R A C T

Titanium-nitrogen complexes were generated by laser ablated titanium (Ti) atoms and N_2 gas molecules in this study. These complexes were isolated on the pre-deposited solid Ar matrix on the pre-cooled KBr window (T ~ 5.4 K), allowing infrared spectra to be measured. Laser ablation experiments with $^{15}N_2$ isotope provided distinct isotopic shifts in the infrared spectra that strongly implicated the formation of titanium-nitrogen complexes, $Ti(NN)_x$. Density functional theory (DFT) calculations were employed to investigate the molecular structures, electronic ground state, relative energies, and IR frequencies of the anticipated $Ti(NN)_x$ complexes. Based on laser ablation experiments and DFT calculations, we were able to assign multiple $Ti(NN)_x$ (x = 1-6) species. Particularly, $Ti(NN)_5$ and $Ti(NN)_6$, which have high nitrogen content, may serve as good precursors in preparing polynitrogens.

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