Towards a comprehensive understanding of the chemical vapor deposition of titanium nitride using $Ti(NMe_2)_4$: a density functional theory approach

Kaushik Sen, Tahamida Banu, Tanay Debnath, Deepanwita Ghosh, and Abhijit K. Das*
Department of Spectroscopy, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, India

Supporting Information

Table S1 Partition functions (Q) used in the calculations of the rate constants and equilibrium constant of the reaction between TDMAT and NH_3

Species	M06L/LANL2DZ			
	Q_{vib}	Q_{trans}	Q_{rot}	Q
$Ti(NMe_2)_4$	3.26E+08	3.24E+33	2.07E+06	2.19E+48
NH_3	1.09E+00	6.79E+31	6.86E+01	5.09E+33
$Ti(NMe_2)_4 \cdot NH_3$ (C6)	2.68E+09	3.62E+33	2.38E+06	2.31E+49
TS7	4.19E+07	3.62E+33	2.38E+06	3.62E+47
$(Me_2N)_3TiNH_2$ (C7)	1.24E+07	2.66E+33	1.37E+06	4.53E+46
TS8	1.57E+06	2.66E+33	1.40E+06	5.83E+45

Table S2 Imaginary frequencies (ν_i) of the transition states involved and Wigner's tunneling correction ($\Gamma(T)$) for the reaction of TDMAT with NH_3

Reaction	TS	ν_i/cm^{-1}	$\Gamma(T)$
$Ti(NMe_2)_4 \cdot NH_3$ (C6) → $(Me_2N)_3TiNH_2$ (C7) + $HNMe_2$	TS7	654*i*	1.416
$(Me_2N)_3TiNH_2$ (C7) → $(Me_2N)_2TiNH$ (C8) + $HNMe_2$	TS8	1544*i*	3.318