

SUPPLEMENTARY MATERIAL

Table 1. Imaginary frequencies (cm^{-1}) calculated for the unbound normal mode in the so-called TS1, TS5 and TS6.

		<i>Imaginary frequencies (in cm^{-1})</i>		
		TS1	TS5	TS6
b3lyp	6-31G*	-811	-912	-705
	cc-pVDZ	-788	-886	-725
mp2	6-31G*	-887	-974	-794
	cc-pVDZ	-802	-891	-680

Table 2. Transmission coefficients calculated using the Wigner approximation for the uncatalyzed (TS1), catalyzed with ammonia (TS5) and catalyzed with OH (TS6), hydrolysis reaction of the TMOS at 273K and 300K.

		<i>Transmission coefficient (at $T=273\text{K}$)</i>			<i>Transmission coefficient (at $T=300\text{K}$)</i>		
		TS1	TS5	TS6	TS1	TS5	TS6
b3lyp	6-31G*	1,019	1,024	1,015	1,016	1,020	1,012
	cc-pVDZ	1,018	1,023	1,015	1,015	1,019	1,013
mp2	6-31G*	1,023	1,028	1,018	1,019	1,023	1,015
	cc-pVDZ	1,019	1,023	1,014	1,016	1,019	1,011