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Supplementary Information

Catalytic Dissociation of Tris(dimethylamino)silane on Hot Tungsten and Tantalum Filament Surfaces

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Table S1. Relative enthalpies (kcal·mol^{-1}), Gibbs free energies (kcal·mol^{-1}) and entropies (cal·mol^{-1}·K^{-1}) of relevant species to the reactants at different temperatures calculated at the CCSD(T)/6-311+G(2d,p)//B3LYP/6-311++G(d,p) level

	P1 + P2[a] Concerted Si-N breakage			R1 + R2[b] Stepwise Si-N cleavage			TS-Si-N-S2[c] Stepwise Si-N cleavage			R1 + R6[d] + P2 Stepwise Si-N cleavage		
Temperature (K (^{0}C))	ΔH	ΔG	ΔS	ΔH	ΔG	ΔS	ΔH	ΔG	ΔS	ΔH	ΔG	ΔS
0 (-273)	36.2	36.2	0	92.3	92.3	0	127.4	127.4	0	123.6	123.6	0
1373 (1100)	33.7	-20.2	39.2	90.7	27.3	46.2	126.0	62.1	46.5	124.2	28.0	70.1
1573 (1300)	33.0	-28.0	38.8	90.0	18.1	45.7	125.1	52.8	46.0	123.5	14.1	69.6
1773 (1500)	32.3	-35.7	38.4	89.3	9.0	45.3	124.2	43.7	45.4	122.8	0.2	69.2
1973 (1700)	31.6	-43.3	38.0	88.6	0.0	44.9	123.2	34.7	44.9	122.0	-13.6	68.7
2073 (1800)	31.3	-47.1	37.8	88.3	-4.5	44.7	122.7	30.2	44.6	121.6	-20.5	68.5
2273 (2000)	30.5	-54.6	37.5	87.5	-13.4	44.4	121.7	21.3	44.2	120.8	-34.1	68.2

[a] P1 and P2 represent bis(dimethylamino) silane and N-methyl methyleneimine (NMMI), respectively;
[b] R1 and R2 represent bis(dimethylamino)silyl and dimethylamino radical, respectively;
[c] TS-Si-N-S2 represents the transition state for the formation of N-methyl methyleneimine (P2) from dimethylamino radical (R2);
[d] R6 represents the H radical.