A theoretical study of the $N_2 + H_2$ reactive collisions for high vibrational and translational energies. Supplementary Material

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Table S1: Fitted coefficients to the model given by Equations (9) - (13) for the reaction $H_2(v'') + N_2(v')$. Units are such that the cross section in Equation (9) comes in Å^2 when energies are in kcal mol^{-1}

v''	v'	a_0	b_0	c_0	d_0	a_1	b_1	c_1	d_1	E_r/kcal mol^{-1}
4	4, 6, 8	3.57419×10^{-9}	0.02809	4.89782	76.4703	3.14423×10^{-11}	-1.39585×10^{-9}	−0.000840399	−0.219901	29.3048
4	10, 12	6.04411×10^{-13}	0.03494	6.82859	43.196	2.48777×10^{-15}	-1.41162×10^{-9}	−0.000840399	−0.219901	77.5067
5	4, 6, 8	7.62308×10^{-10}	0.0271106	5.1576	44.9172	4.05202×10^{-12}	-1.3982×10^{-9}	−0.000840399	−0.219901	29.3048
5	12	4.43611×10^{-14}	0.0445261	7.67707	31.3991	2.28779×10^{-17}	-1.41162×10^{-9}	−0.000840399	−0.219901	77.5067
6	0 – 12	3.19893×10^{-5}	0.0246831	2.87158	54.58	1.86344×10^{-7}	−0.000144581	−0.00246571	−0.080389	3.3276
8	0 – 12	0.0153365	0.00751311	1.36855	33.4306	-5.90881×10^{-5}	-4.41426×10^{-5}	0.000705679	−0.061483	3.3276
10	0 – 12	0.210423	0.00743152	0.973406	18.8643	0.000691641	-2.36879×10^{-5}	−0.000785404	0.00320755	3.3276
12	0 - 12	3.25233	0.00510684	0.440203	9.0369	0.0158256	-2.52828×10^{-5}	−0.00126669	0.00653197	3.3276

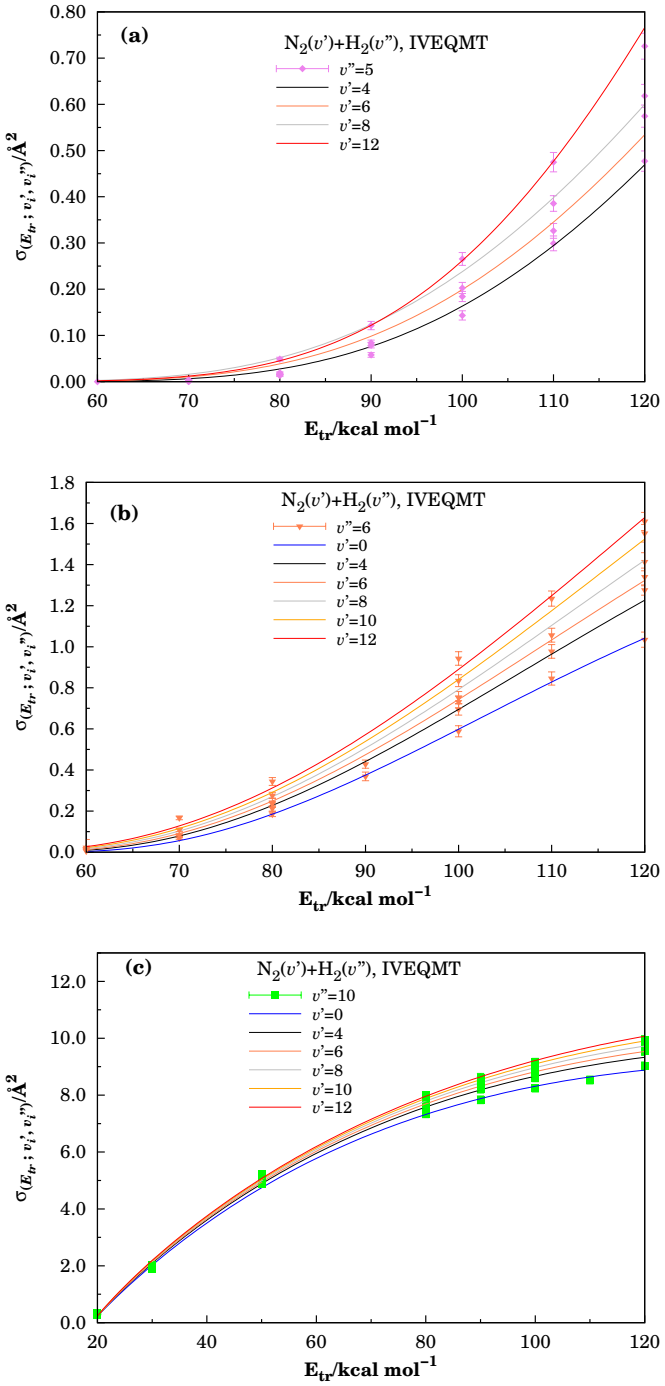

Figure S1: Specific initial-state cross section for the reaction $N_2(v') + H_2(v'') \rightarrow N_2 + H + H$ considering the IVEQMT approach. In Panel (a) $H_2(v'' = 5) + N_2(v' = 4, 6, 8, 12)$, in Panel (b) $H_2(v'' = 6) + N_2(v' = 0, 4, 6, 8, 10, 12)$ and in Panel (c) $H_2(v'' = 10) + N_2(v' = 0, 4, 6, 8, 10, 12)$,

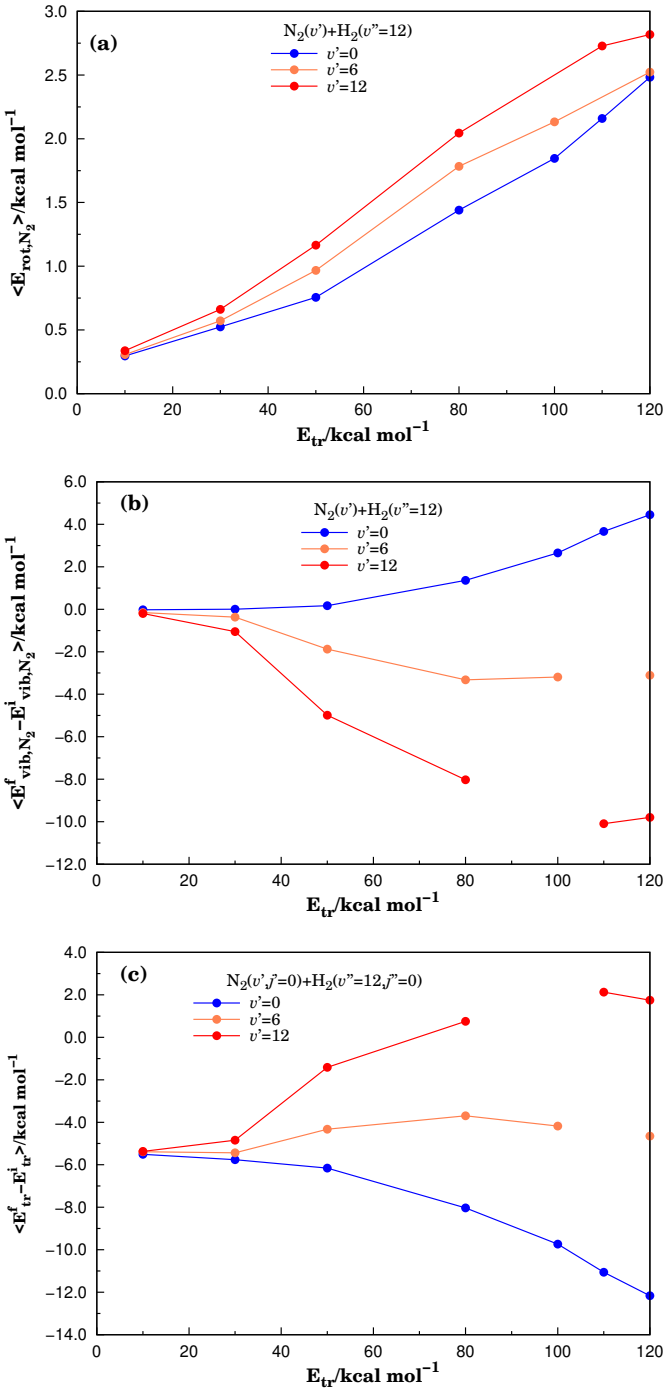

Figure S2: Comparison of the arithmetic mean of energies for different degrees of freedom in the reaction $N_2(v' = 0, 6, 12) + H_2(v'' = 12) \rightarrow N_2 + H + H$ within the IVEQMT approach versus translational energies. In Panel (a) are displayed the mean values of the rotational energy for the product N_2. In Panel (b) the differences between the mean values of the vibrational energy for the N_2 after reaction and the corresponding initial value are shown. In Panel (c) the difference between mean values of the relative translational energy of the molecular system after reaction and the corresponding initial values are presented.

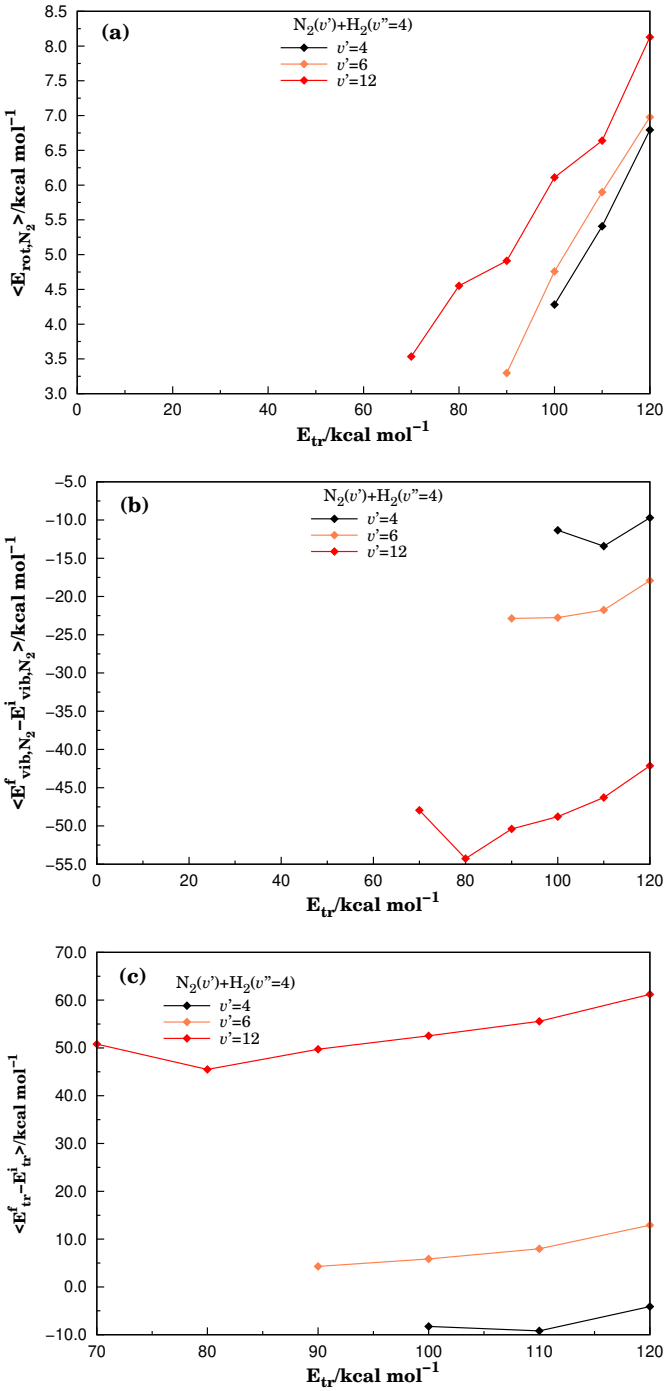

Figure S3: Comparison of the arithmetic mean of energies for different degrees of freedom in the reaction $N_2(v' = 4, 6, 12) + H_2(v'' = 4) \rightarrow N_2 + H + H$ within the IVEQMT approach versus translational energies. In Panel (a) are displayed the mean values of the rotational energy for the product N_2. In Panel (b) the differences between the mean values of the vibrational energy for the N_2 after reaction and the corresponding initial value are shown. In Panel (c) the difference between mean values of the relative translational energy of the molecular system after reaction and the corresponding initial values are presented.

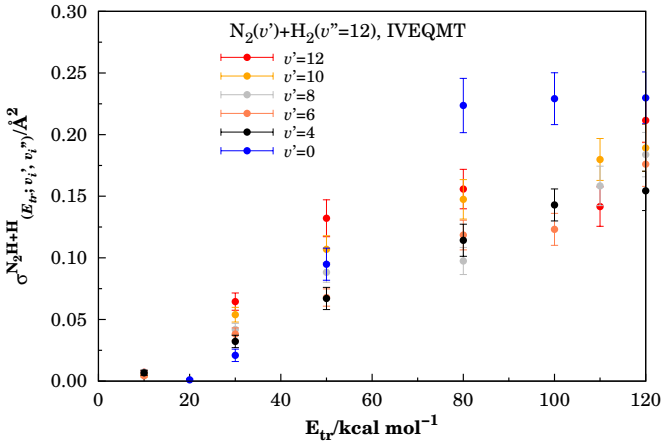

Figure S4: Specific initial-state reactive cross section for the $N_2H + H$ formation considering the reactive collisions $H_2(v'' = 12)$+$N_2(v' = 0, 4, 6, 8, 10, 12)$ in the frame of the IVEQMT approach.