Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering.

Supplementary Material for

An optimized model for ammonia/syngas combustion

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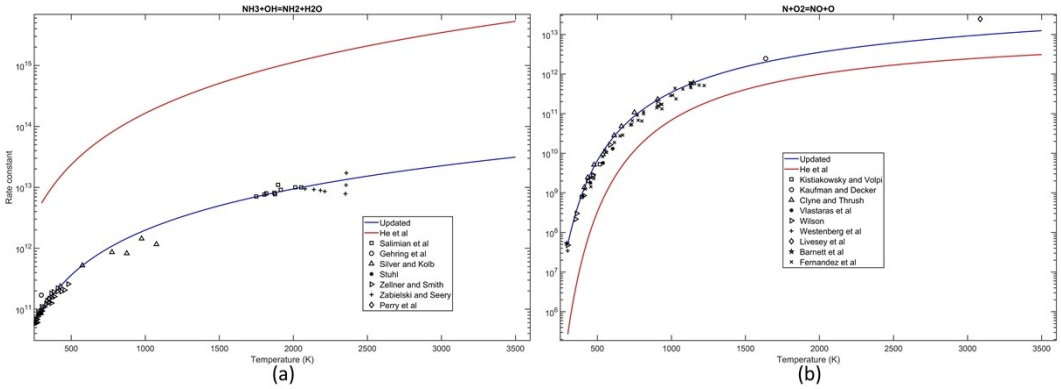


Figure S1. Rate constants of (a) NH_3+OH=NH_2+H_2O measured by Salimian et al. [1], Gehring et al. [2], Silver and Kolb [3], Stuhl [4], Zellner and Smith [5], Zabielski and Seery [6] and Perry et al.[7], and (b) N+O2=NO+O measured by Kistiakowsky and Volpi [8], Kaufman and Decker [9], Clyne and Thrush [10], Vlastaras et al. [11], Wilson [12], Westenberg et al. [13], Livesey et al. [14], Barnett et al. [15] and Fernandez et al. [16], and those predicted using the updated (blue) and original (red) rate parameters.

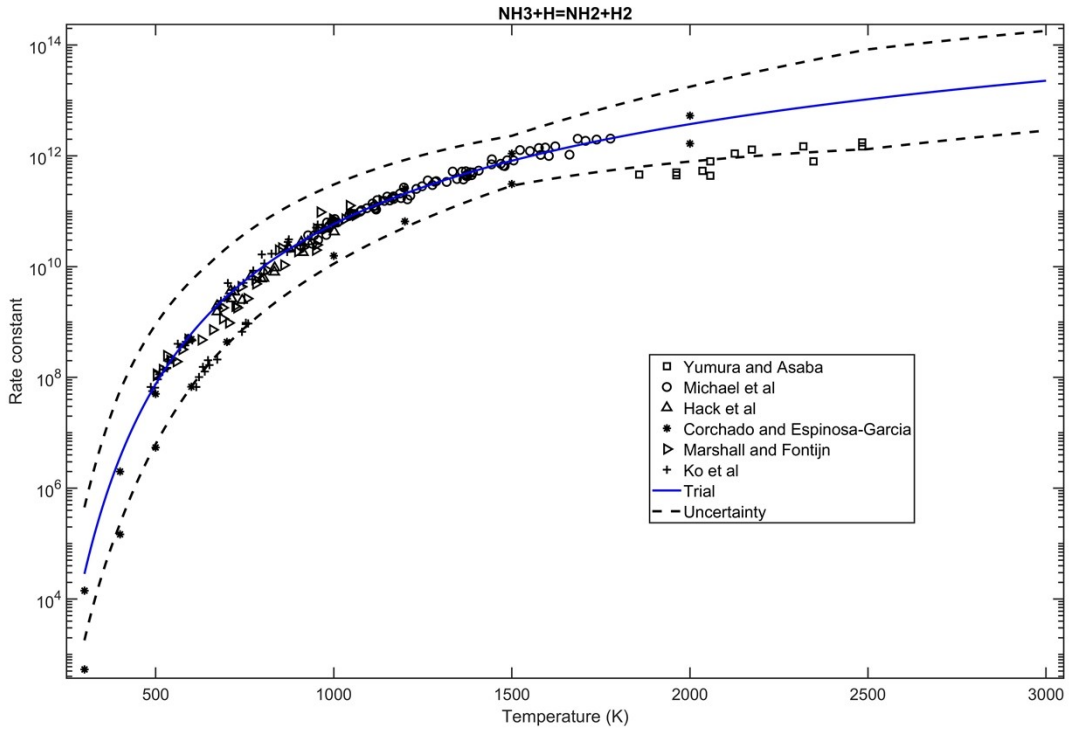


Figure S2. Rate constant of NH_3+H=NH_2+H_2 in the trial model and the uncertainty factor estimated based on available experimental data of Yumura and Asaba [17], Michael et al. [18], Hack et al. [19], Corchado and Espinosa-Garćia [20], Marshall and Fontijn [21] and Ko et al. [22].

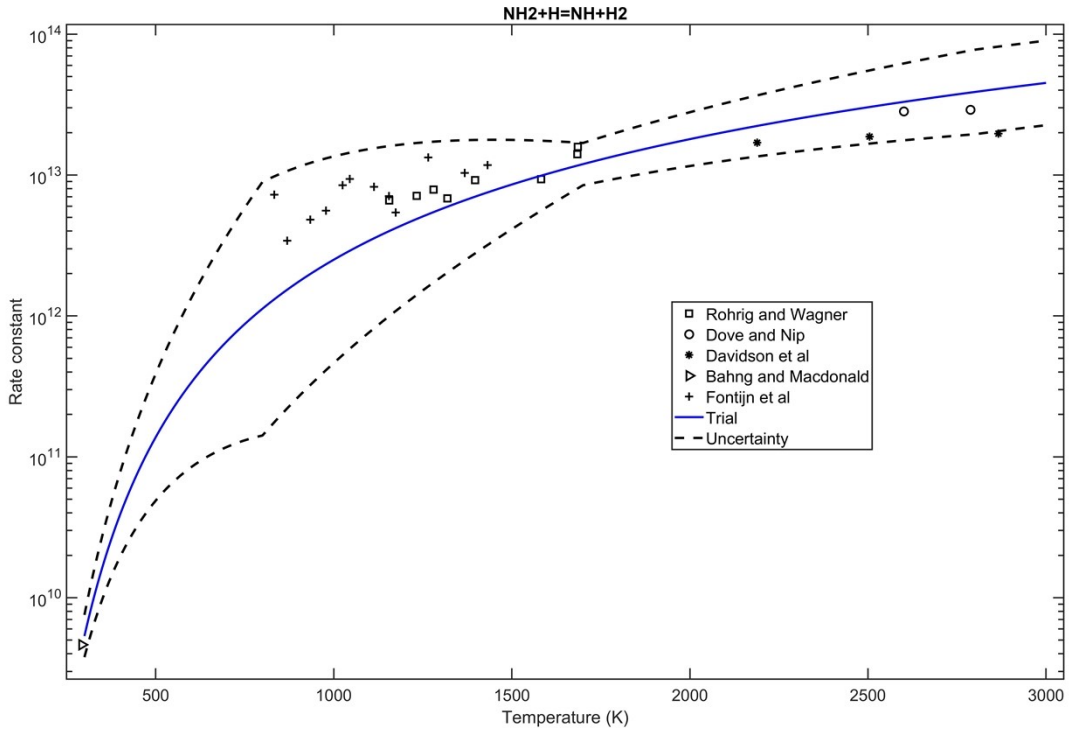


Figure S3. Rate constant of NH_2+H=NH+H_2 in the trial model and the uncertainty factor estimated based on available experimental data of Röhrig and Wagner [23], Dove and Nip [24], Davidson et

al. [25], Bahng and Macdonald [26] and Fontijn et al. [27].

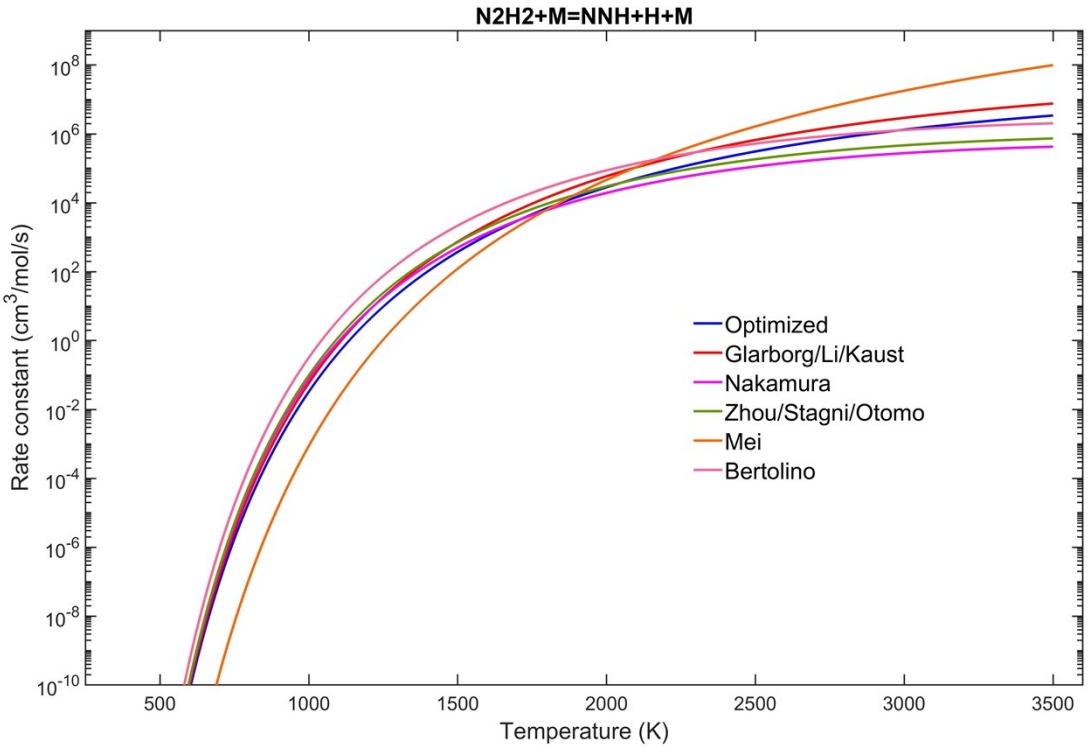


Figure S4. Rate constant of N_2H_2+M=NNH+H+M predicted using the investigated models.

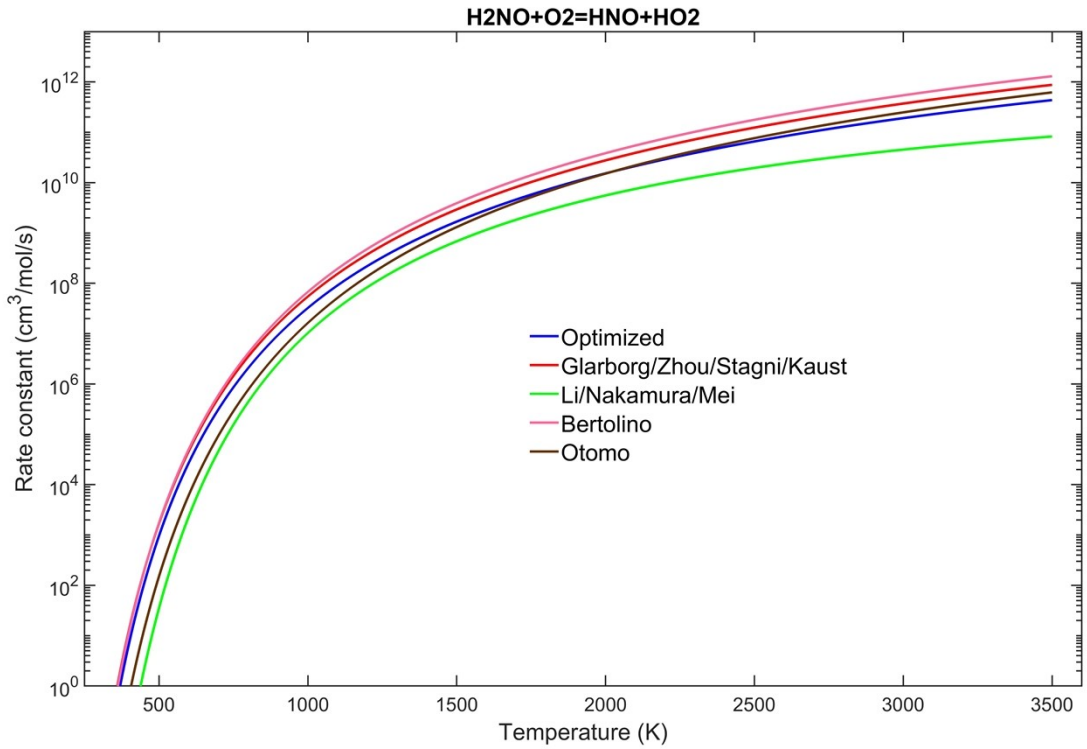


Figure S5. Rate constant of $H_2NO+O_2=HNO+HO_2$ predicted using the investigated models.

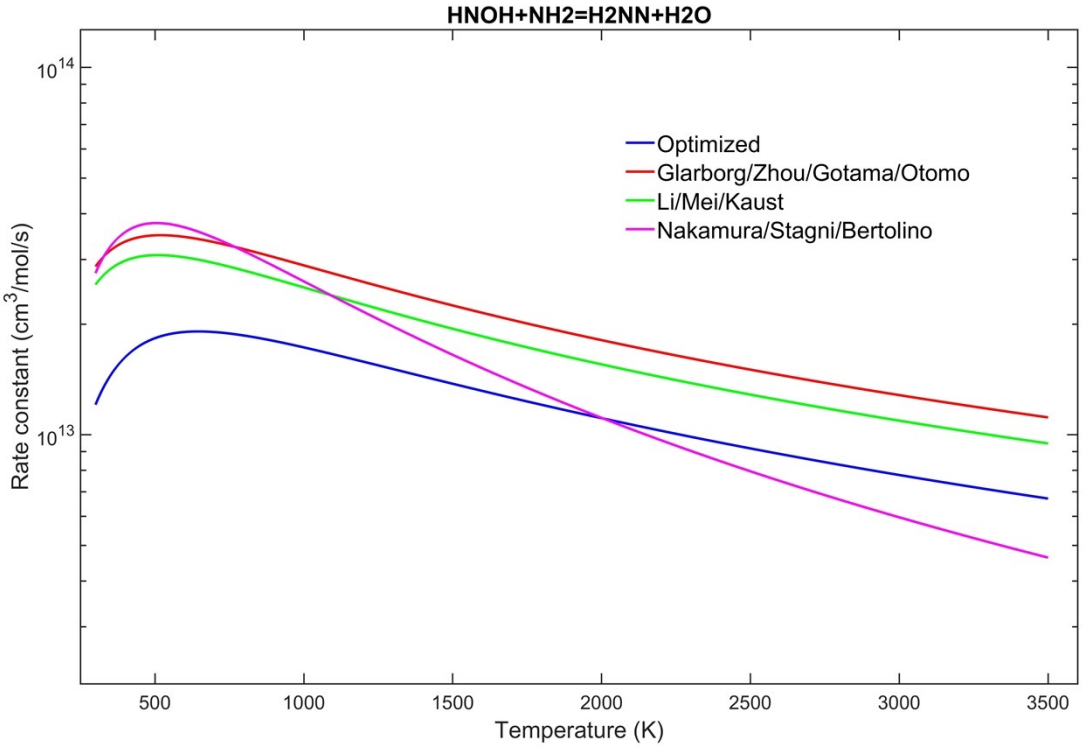


Figure S6. Rate constant of $HNOH+NH_2=H_2NN+H_2O$ predicted using the investigated models.

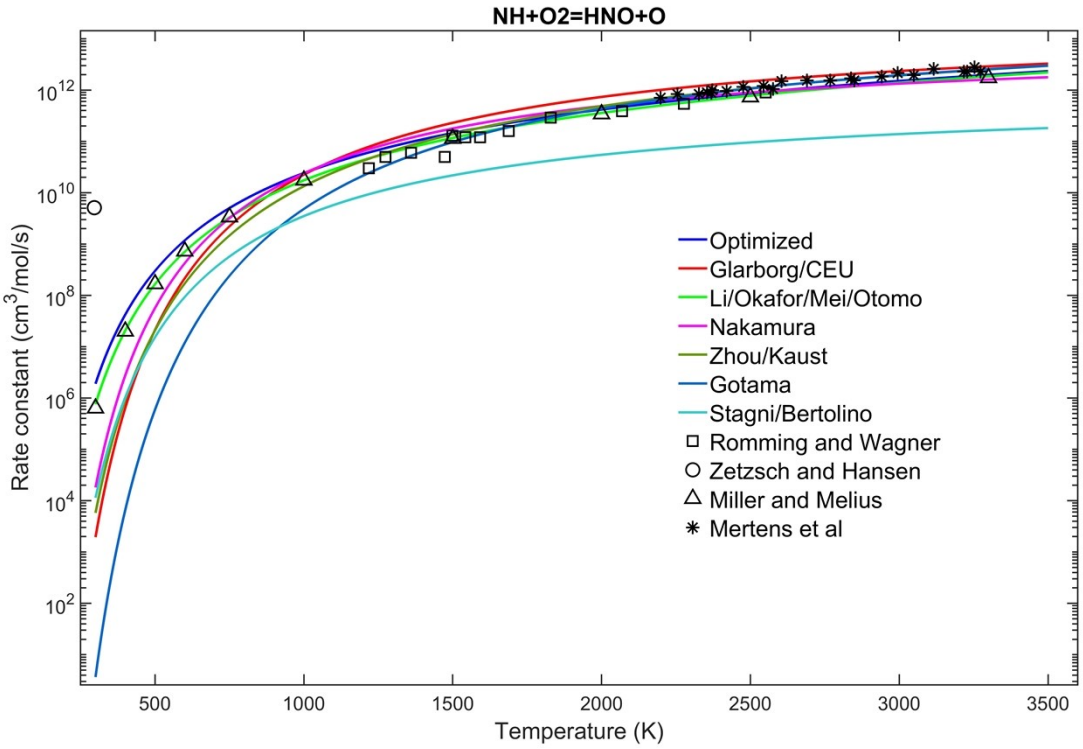


Figure S7. Rate constant of NH+O2=HNO+O predicted using the investigated models and the experimental data of Römming and Wagner [28], Zetzsch and Hansen [29], Miller and Melius [30] and Mertens et al. [31].

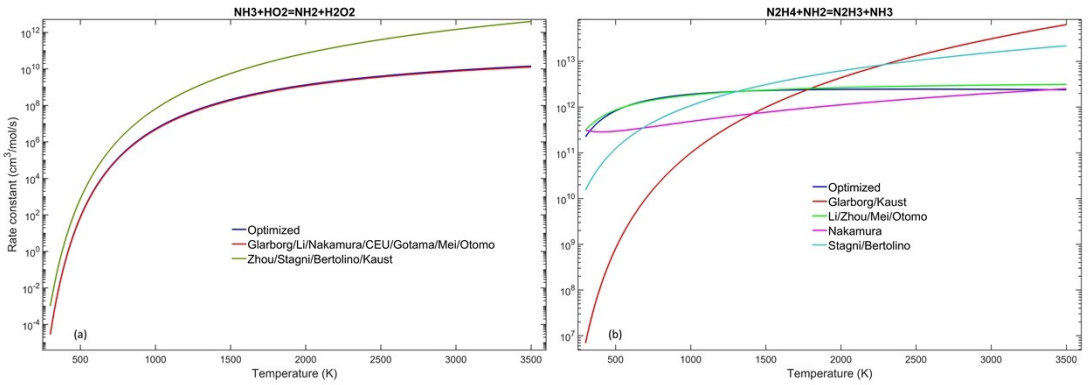


Figure S8. Rate constant of (a) $NH_3+HO_2=NH_2+H_2O_2$ and (b) $N_2H_4+NH_2=N_2H_3+NH_3$ predicted using the investigated models.

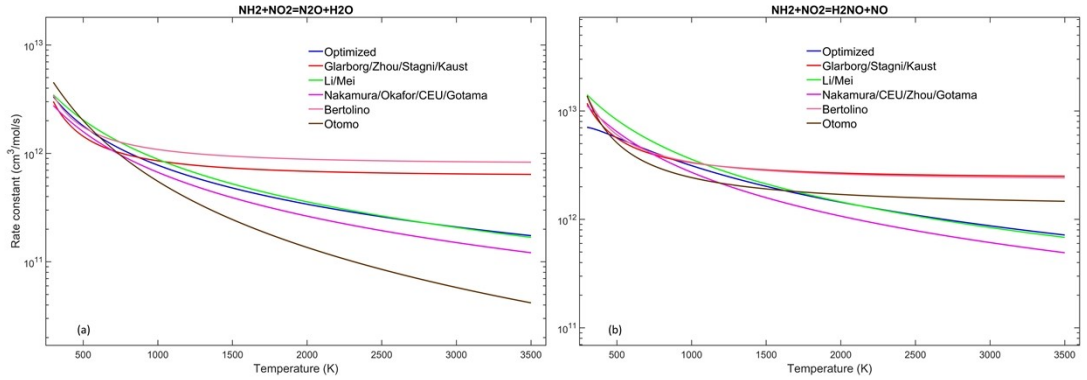


Figure S9. Rate constant of (a) $NH_2+NO_2=N_2O+H_2O$ and (b) $NH_2+NO_2=H_2NO+NO$ predicted using the investigated models.

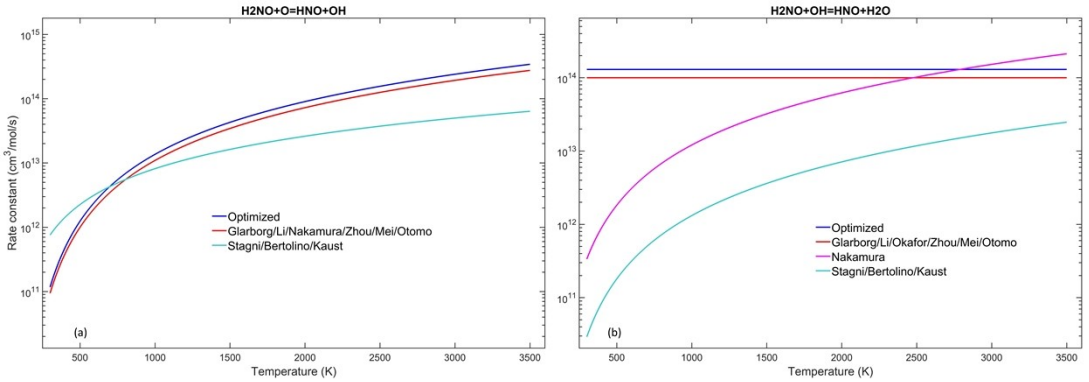


Figure S10. Rate constant of (a) $H_2NO+O=HNO+OH$ and (b) $H_2NO+OH=HNO+H_2O$ predicted using the investigated models.

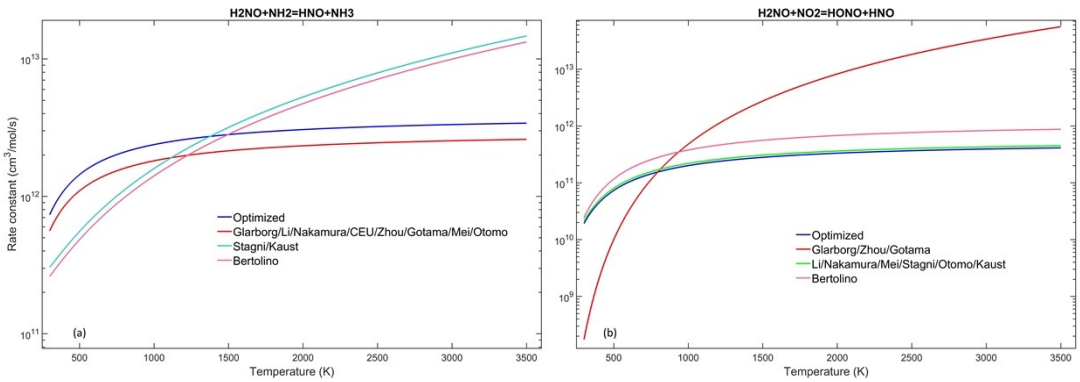


Figure S11. Rate constant of (a) $H_2NO+NH_2=HNO+NH_3$ and (b) $H_2NO+NO_2=HONO+HNO$ predicted using the investigated models.

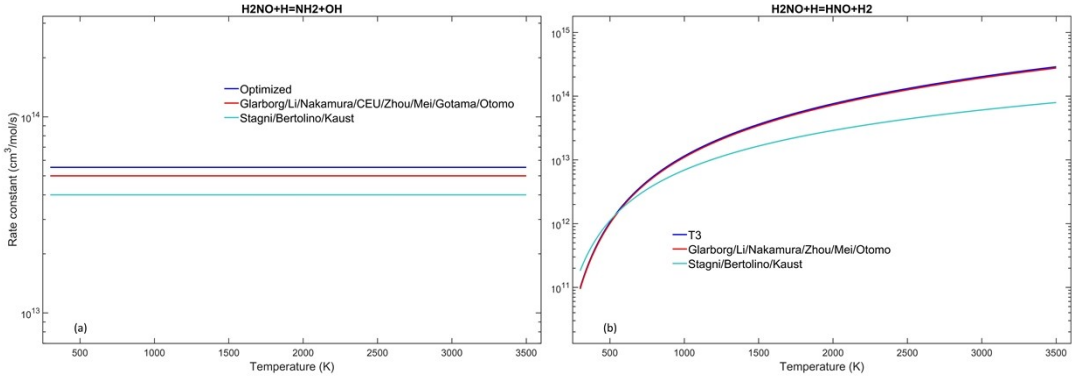


Figure S12. Rate constant of (a) $H_2NO+H=NH_2+OH$ and (b) $H_2NO+H=HNO+H_2$ predicted using the investigated models.

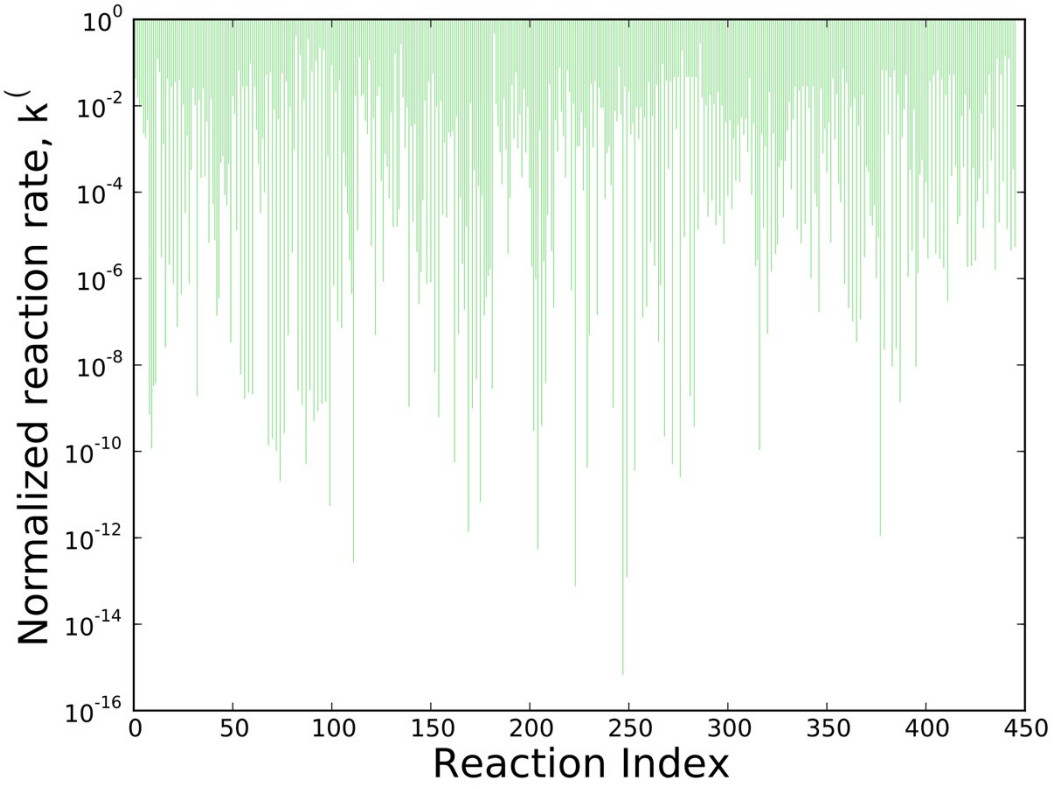
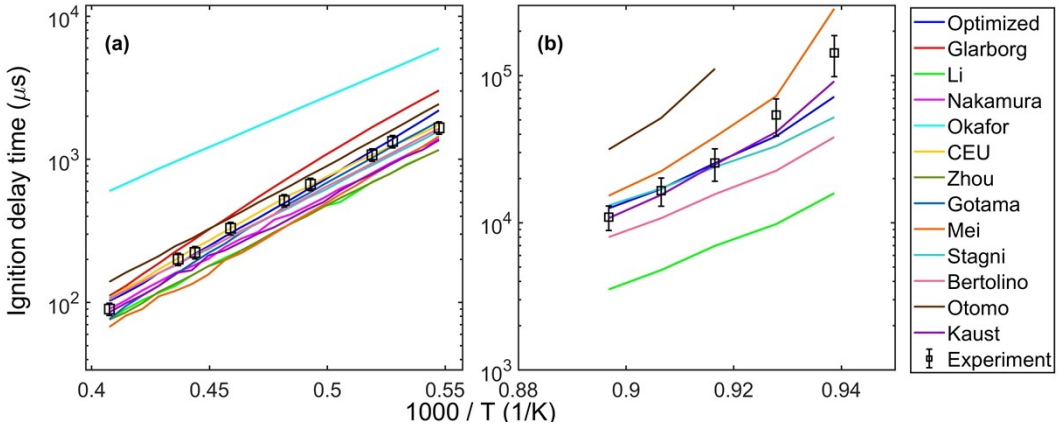


Figure S13. Distribution of normalized reaction rate of reactions in the optimized model. Reaction rates are calculated separately for forward and reverse directions for reversable reactions. Values smaller than 1 indicate no violation of collision limit.



Figures S14. Simulation results for the ignition delay time measurements reported by (a) Mathieu and Petersen [32] and (b) He et al. [33] using the investigated models. The experimental and simulation condition in (a) is stoichiometric NH_3/O_2 mixtures diluted in 98% Ar at 1.4 atm. The experimental and simulation condition in (b) is NH_3/O_2/Ar=0.12/0.18/0.7 mixtures at 40 bar after compression.

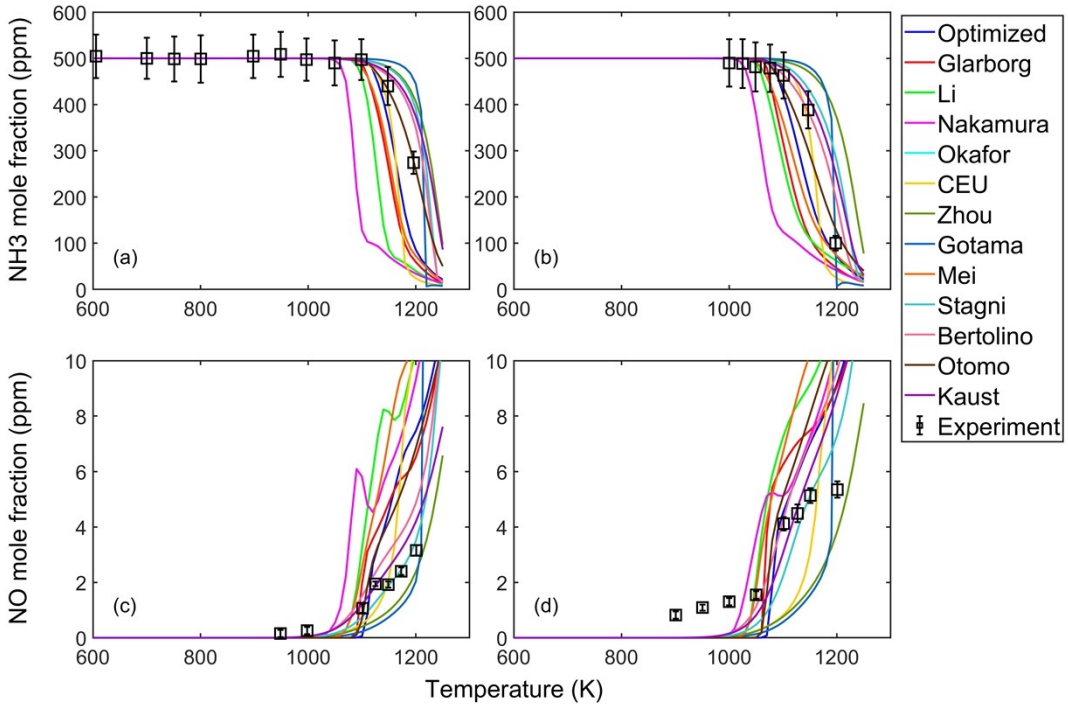


Figure S15. Simulation results of the NH_3 and NO data measured by Stagni et al. [34]. The experimental conditions are (a) and (c) 500 ppm NH_3 and 2% O_2 diluted in He at 800 torr, (b) and (d) 500 ppm NH_3 and 4% O_2 diluted in He at 800 torr. The residence time is 1.5s for all cases.

Table S1. Ammonia ignition delay time experiments used in the current study.

Number of measurements	Mixture	Equivalence ratio	Pressure (atm)	Temperature (K)	Uncertainty
Mathieu et al. (2015) [32]; ignition criterial: d[OH*]/dt maximum					
104	$NH_3/O_2/Ar$	0.5-2.0	1.25-30.4	1564-2489	10%
Shu et al. (2019) [35]; ignition criteria: dP/dt maximum					
30	NH_3/air	0.5-2.0	15.9-41.6	1181-1581	20%
Chen et al. (2021) [36]; ignition criteria: d[OH*]/dt maximum					
66	$NH_3/H_2/O_2/Ar$	1	1.01-12.6	1022-1956.9	20%
He et al. (2019) [33]; ignition criteria: dP/dt maximum					
84	$NH_3/H_2/O_2/Ar/N_2$	0.5-2.0	19.5-59.8	969.4-1130.6	15%-55%
Dai et al. (2020) [37]; ignition criteria: dP/dt maximum					
88	$NH_3/H_2/O_2/Ar/N_2$	0.5-3.0	19.5-72.6	955.5-1205	8.8%-25.2%

Table S2. Ammonia laminar flame speed experiments used in the current study.

Number of measurements	Fuel	Diluent	Equivalence ratio	Temperature (atm)	Pressure (K)	Uncertainty
Lhuillier et al. (2020) [38]						
265	NH_3, H_2	N_2	0.8-1.4	298-473	0.99	10.8%-

						68.2%
Ronney (1988) [39]						
71	NH_3	N_2	0.7-1.65	298	0.06-1.97	15%
Han et al. (20169) [40]						
216	NH_3, H_2, CO	N_2	0.7-1.7	298	1	1%-33.3%
Han et al. (2020) [41]						
172	NH_3, H_2, CO	N_2	0.7-1.6	298	1	1%-10.8%
Mei et al. (2021) [42]						
9	NH_3	NO	1.1-1.9	298	1	7.2%-10.5%
Takizawa et al. (2008) [43]						
7	NH_3	N_2	0.9-1.2	298	1.05	25%
Ichikawa et al. (2015) [44]						
21	NH_3, H_2	N_2	1.0	298	0.99-4.93	15%
Hayakawa et al. (2015) [45]						
13	NH_3	N_2	0.8-1.2	298	0.99-4.93	3%-24.2%
Pfahl et al. (2000) [46]						
46	NH_3, H_2	N_2	0.44-4.5	298	0.09-0.61	15%
Mei et al. (2020) [47]						
100	NH_3, H_2, CO	N_2	0.7-1.5	298	1-10	2.7%-10.2%
Liu et al. (2019) [48]						
24	NH_3	N/A	0.5-1.75	298	0.5-1.6	20%
Mei et al. (2019) [49]						
51	NH_3	N_2	0.6-1.5	298	1-5	3%-15.5%
Wang et al. (2020) [50]						
51	NH_3	N_2	0.6-1.4	303-393	0.99	6.9%-15.9%
Wang et al. (2020) [51]						
289	NH_3, H_2, CO	N_2	0.6-1.6	298	0.99-4.9	1.5%-15.2%
Lee et al. (2010) [52]						
10	NH_3, H_2	N_2	0.62-0.73	298	1	15%
Li et al. (2014) [53]						
66	NH_3, H_2	N_2	0.6-1.37	298	1	20%

Table S3. List of the influential reactions and their estimated uncertainty function $f(T)$.

Reaction	$f(T)$	Estimation approach	Source
HNO+OH=NO+H2O	0.48 between 300 K and 3000 K	Based on review literature	[54]
HNO+O2=HO2+NO	0.5 between 300 K and 3000 K	Based on Bertolino rules	[55]
NO+H(+M)=HNO+M	0.5 at 400 K, increasing to 0.55 at 900 K, increasing to 1.00 at 2000 K	Based on uncertainty quantification work	[56]
N2O(+M)=N2+O(+M)	1 at 700 K, decreasing to 0.75 at 1200 K, increasing to 1 at 3200 K	Based on uncertainty quantification work	[56]
N2O+H=N2+OH	1.60 at 500 K, decreasing to 0.70	Based on uncertainty	[56]

	at 1200 K, increasing to 0.60 at 2600 K	quantification work	
NH2+H(+M)=NH3(+M)	0.4 between 2000 K and 3000 K	Based on review literature	[57]
NH3+H=NH2+H2	1.2 at 400 K, increasing to 0.9 at 650 K, decreasing to 0.45 at 1500 K, increasing to 0.9 at 2500 K	Based on experimental measurements (see Fig. S2)	[17-22]
NH3+HO2=NH2+H2O2	0.7 between 300 K and 3000 K	Based on domain knowledge	[58]
NH2+H=NH+H2	0.15 at 300 K, increasing to 0.9 at 800 K, decreasing to 0.15 at 1700 K, increasing to 0.3 at 2800 K	Based on experimental measurements (see Fig. S3)	[23-27]
NH2+O=HNO+H	0.7 between 300 K and 3000 K	Based on domain knowledge	[59]
NH2+HO2=H2NO+OH	1.0 between 300 K and 3000 K	Based on Bertolino rules	[60]
NH2+O2=H2NO+O	0.3 between 300 K and 3000 K	Based on Bertolino rules	[61]
NH2+NH=N2H2+H	0.7 between 300 K and 3000 K	Based on Bertolino rules	[62]
NH2+NO=N2+H2O	0.3 between 298 K and 1200 K, increasing to 0.5 between 2000 K and 3300 K	Based on review literature	[57]
NH2+NO=NNH+OH	0.3 between 298 K and 1200 K, increasing to 0.5 between 2000 K and 3300 K	Based on review literature	[57]
NH2+HONO=NH3+NO2	0.7 between 300 K and 3000 K	Based on Bertolino rules	[63]
NH2+NO2=N2O+H2O	0.7 between 300 K and 3000 K	Based on domain knowledge	[64]
NH2+NO2=H2NO+NO	0.7 between 300 K and 3000 K	Based on domain knowledge	[64]
NH+O2=HNO+O	0.7 between 300 K and 3000 K	Based on domain knowledge	[30]
NH+NO=N2O+H	0.3 between 300 K and 3000 K	Based on Bertolino rules	[61]
N+NO=N2+O	0.2 between 300 K and 3000 K	Based on review literature	[65]
NH2+NH2(+M)=N2H4(+M)	0.3 between 300 K and 3000 K	Based on Bertolino rules	[66]
N2H4+NH2=N2H3+NH3	0.7 between 300 K and 3000 K	Based on domain knowledge	[59]
N2H3+M=N2H2+H+M	0.5 between 300 K and 3000 K	Based on Bertolino rules	[55]
N2H3+HO2=N2H4+O2	0.5 between 300 K and 3000 K	Based on Bertolino rules	[55]
N2H3+NH2=H2NN+NH3	0.5 between 300 K and 3000 K	Based on Bertolino rules	[55]
N2H2+M=NNH+H+M	0.7 between 300 K and 3000 K	Based on Bertolino rules	[62]
N2H2+H=NNH+H2	0.7 between 300 K and 3000 K	Based on Bertolino	[62]

		rules	
N2H2+NO=N2O+NH2	0.5 between 300 K and 3000 K	Based on Bertolino rules	[55]
NH2+NH2=N2H2+H2	0.3 between 300 K and 3000 K	Based on Bertolino rules	[66]
H2NN=N2+H2	0.5 between 300 K and 3000 K	Based on Bertolino rules	[55]
H2NN+O2=NH2+NO2	0.5 between 300 K and 3000 K	Based on Bertolino rules	[55]
H2NO+HO2=HNO+H2O2	0.5 between 300 K and 3000 K	Based on Bertolino rules	[55]
H2NO+O2=HNO+HO2	0.6 between 300 K and 3000 K	Based on Bertolino rules	[67]
HNOH+NH2=H2NN+H2O	0.5 between 300 K and 3000 K	Based on Bertolino rules	[55]
H2NO+NH2=HNO+NH3	0.7 between 300 K and 3000 K	Based on domain knowledge	[68]
H2NO+H=HNO+H2	0.7 between 300 K and 3000 K	Based on domain knowledge	[68]
H2NO+H=NH2+OH	0.7 between 300 K and 3000 K	Based on domain knowledge	[68]
H2NO+O=HNO+OH	0.7 between 300 K and 3000 K	Based on domain knowledge	[68]
H2NO+OH=HNO+H2O	0.7 between 300 K and 3000 K	Based on domain knowledge	[68]
H2NO+NO2=HONO+HNO	0.7 between 300 K and 3000 K	Based on domain knowledge	[68]

*Uncertainty factor was interpreted as a piece-wise linear function between the reported temperature nodes and a constant outside the reported temperature range

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