Thermochemical production of ammonia via a two-step metal nitride cycle – Materials screening and the Strontium-based system

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Supplementary Information

1. Theoretical Screening

1.1 Formulation

Data was obtained from the Materials Project database (MP, database version: v2023.11.1)[1]. The Python library pymatgen (Python Material Genomics)[2] was used for the calculations. The essential data exported were the energy above convex hull per atom E_{hull}, the formation energy per atom E_{form}, and the elastic tensor c_{ij}.

The calculation of the heat capacity is based on the Debye model.[3,4] Longitudinal and transverse sound velocities v_l and v_t are calculated with the pymatgen functions `long_v` and `trans_v` which use the Voigt-Reuss-Hill average bulk modulus derived from the elastic tensor c_{ij}. The volume of the primitive cell v_0 is

$$v_0 = \frac{v}{n_{sites}} \tag{S1}$$

where v is the volume of the conventional unit cell and n_{sites} the number of sites in the unit cell. The average sound velocity v_m is defined as

$$v_m = \left(\frac{3}{\frac{1}{v_l^3} + \frac{2}{v_t^3}} \right)^{1/3} \tag{S2}$$

The Debye temperature Θ_D is given as

$$\Theta_D = \frac{\hbar}{k_B} v_m \left(\frac{6\pi^2}{v_0} \right)^{1/3} \tag{S3}$$

where $\hbar$ is the reduced Planck constant and k_B is the Boltzmann constant. The specific heat capacity at constant volume c_v can then be approximated as

$$c_v(T) = 9R \cdot n \cdot \left(\frac{T}{\Theta_D} \right)^3 \int_0^{\Theta_D/T} \frac{x^4 \cdot e^x}{(e^x - 1)^2} dx \tag{S4}$$

where n is the number of atoms and T is the temperature in Kelvin. With the assumption that the heat capacity ratio of a solid is nearly 1, the specific heat capacity at constant pressure c_p is approximated as:

$$c_p(T) = c_v(T) \tag{S5}$$

The entropy is directly calculated from the approximation of the specific heat capacity as:

$$s(T) = \int_{0\,K}^{T} \frac{c_p}{T} dT \tag{S6}$$

The standard enthalpy of formation h_f^o is approximated with the help of the formation energy per atom E_{form}:

$$h_f^o = E_{form} \cdot e \cdot N_A \cdot n \tag{S7}$$

The enthalpy is then calculated as:

$$h(T) = h_f^o + \int_{298\,K}^{T} c_p dT \tag{S8}$$

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1.2 Validation of Thermodynamic Data Approximation

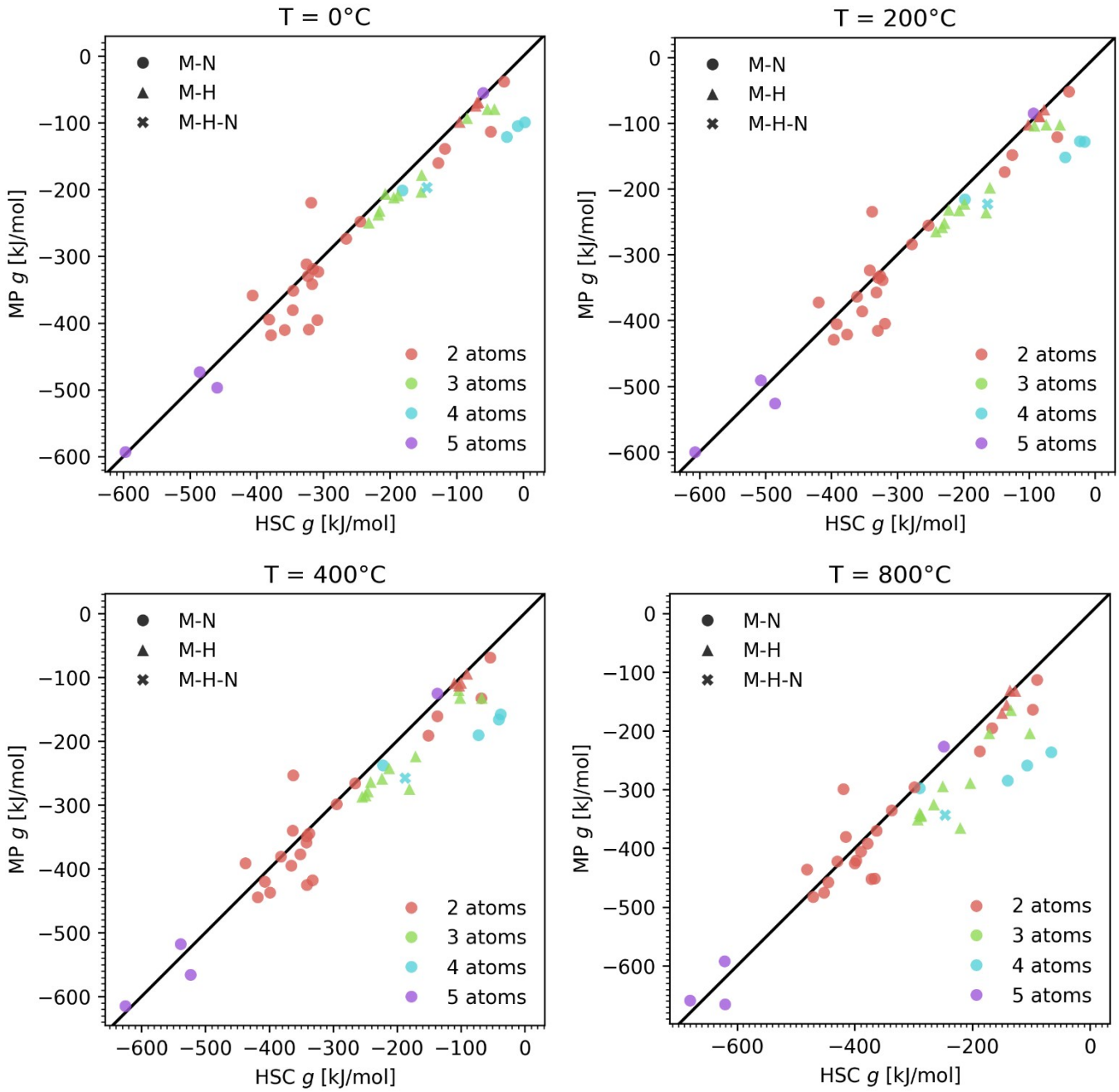

Figure S1: Comparison of Gibbs free energies calculated from MP database data, and Gibbs free energies taken from HSC database for 4 temperatures 0, 200, 400, 800 °C. The shape of the markers indicate the 3 type of materials: metal nitride (M-N), metal hydride (M-H), and metal imide (M-H-N). The color of the markers indicate the number of atoms (some MP data is calculated in eV/atom). The comparison included all available materials that were found in a stable form in both databases: 28 metal nitrides, 15 metal hydrides, 1 metal imide.

1.3 Source of thermodynamic data

Thermodynamic data was obtained from the Materials Project database (MP, database version: v2023.11.1) and from the HSC Chemistry 5 database (HSC). Some materials from the MP database were only used for the calculate of the stoichiometric weight changes since not all required properties for the calculations in Section 1.1 were available (marked with *). When data was available from both databases, HSC data was given preference. The MP data was still used for validation purposes (marked with **).

Table S1: The Al-based system

Formula	Source	mpid	E_hull [eV/atom]	E_form [eV/atom]	n
Al	HSC	-	-	-	-
Al3H*	MP	mp-1183138	0.413076	0.388532	4
AlH12*	MP	mp-1214891	0.12337	0.100714	13
AlH3	HSC	-	-	-	-
AlH6*	MP	mp-1214861	1.008702	0.966626	7

AlN	HSC	-	-	-	-
AlN**	MP	mp-661	0	-1.67967	2

Table S2: The Ca-based system

Formula	Source	mpid	E_hull [eV/atom]	E_form [eV/atom]	n
Ca	HSC	-	-	-	-
CaH2	HSC	-	-	-	-
CaH2**	MP	mp-23713	0	-0.66688	3
Ca(H2N)2*	MP	mp-644307	0	-0.6897	7
Ca16HN8*	MP	mp-675153	0.029588	-0.8758	25
Ca2HN*	MP	mp-24119	0	-0.94564	4
Ca8H3N4*	MP	mp-530696	0.05222	-0.88383	15
CaHN*	MP	mp-34932	0	-0.89293	3
Ca11N8*	MP	mp-680640	0.201076	-0.73335	19
Ca2N	MP	mp-2686	0	-0.89772	3
Ca3N2	HSC	-	-	-	-
Ca3N2**	MP	mp-844	0	-0.95972	5
CaN*	MP	mp-1058549	0.398168	-0.44138	2
CaN2	MP	mp-1009657	0	-0.63927	3
CaN6	MP	mp-676	0.040613	-0.23336	7

Table S3: The Co-based system

Formula	Source	mpid	E_hull [eV/atom]	E_form [eV/atom]	n
Co	HSC	-	-	-	-
Co3H	MP	mp-1025425	0.004233	-0.02174	4
Co4H*	MP	mp-1226072	0.012287	-0.00849	5
CoH*	MP	mp-1206874	0	-0.05194	2
CoH3*	MP	mp-1183678	0.153299	0.127328	4
Co2N	MP	mp-22631	0.177865	0.177865	3
Co3N	HSC	-	-	-	-
Co3N**	MP	mp-1205986	0.159141	0.159141	4
Co4N*	MP	mp-1206425	0.069595	0.069595	5
CoN	MP	mp-448	0.102861	0.102861	2
CoN12*	MP	mp-1194075	1.244613	1.244613	13
CoN3*	MP	mp-22762	0.383968	0.383968	4

Table S4: The Cr-based system

Formula	Source	mpid	E_hull [eV/atom]	E_form [eV/atom]	n
Cr	HSC	-	-	-	-
Cr3H*	MP	mp-1183723	0.757946	0.757946	4
CrH	MP	mp-24669	0.1659	0.1659	2
CrH2*	MP	mp-24208	0.00228	0.00228	3
CrH3*	MP	mp-1183679	0.123355	0.123355	4
Cr2N	HSC	-	-	-	-
Cr2N**	MP	mp-8780	0.244667	-0.25479	3
Cr3N2	MP	mp-1014303	0.087926	-0.51142	5
Cr3N4	MP	mp-1014460	0.277954	-0.36421	7

CrN	HSC	-	-	-	-
CrN**	MP	mp-2132	0	-0.74919	2
CrN2	MP	mp-1014993	0.296759	-0.2027	3

Table S5: The Cu-based system

Formula	**Source**	**mpid**	**E_hull [eV/atom]**	**E_form [eV/atom]**	**n**
Cu	HSC	-	-	-	-
CuH	MP	mp-24093	0.115168	0.115168	2
Cu10N3*	MP	mp-1225831	0.197459	0.197459	13
Cu2N*	MP	mp-1147700	0.351218	0.351218	3
Cu3N	MP	mp-1933	0.19208	0.19208	4
CuN	MP	mp-13117	0.795979	0.795979	2
CuN3	MP	mp-27954	0.293795	0.293795	4
CuN6	MP	mp-608366	0.339206	0.339206	7
CuN8*	MP	mp-1198545	1.244581	1.244581	9

Table S6: The Fe-based system

Formula	**Source**	**mpid**	**E_hull [eV/atom]**	**E_form [eV/atom]**	**n**
Fe	HSC	-	-	-	-
Fe3H*	MP	mp-984102	0.600378	0.566751	4
FeH	MP	mp-1009077	0	-0.06726	2
FeH3	MP	mp-1018061	0.182623	0.148996	4
FeH4*	MP	mp-1079939	0.243415	0.216513	5
Fe12N5*	MP	mp-27908	0.026315	-0.15899	17
Fe24N11*	MP	mp-684887	0.049817	-0.14807	35
Fe2N	HSC	-	-	-	-
Fe2N**	MP	mp-21476	0.056841	-0.15293	3
Fe3N	MP	mp-1804	0	-0.15778	4
Fe4N	HSC	-	-	-	-
Fe4N**	MP	mp-535	0.069992	-0.05623	5
Fe8N	MP	mp-555	0.001092	-0.06903	9
Fe8N3	MP	mp-673174	0.017508	-0.15445	11
FeN	MP	mp-6988	0	-0.31375	2
FeN2*	MP	mp-1080202	0.148476	-0.06069	3

Table S7: The Li-based system

Formula	**Source**	**mpid**	**E_hull [eV/atom]**	**E_form [eV/atom]**	**n**
Li	HSC	-	-	-	-
LiH	HSC	-	-	-	-
LiH**	MP	mp-23703	0	-0.48936	2
Li(H3N)4*	MP	mp-707454	0.02814	-0.41663	17
Li15H9N8*	MP	mp-1201065	0.005666	-0.5779	32
Li2HN*	MP	mp-1189725	0	-0.58257	4
Li3(HN)2*	MP	mp-1210795	0.184018	-0.38728	7
Li3H3N2*	MP	mp-977164	0.0236	-0.56295	8
Li4HN*	MP	mp-30228	0	-0.4702	6
Li7H5N4*	MP	mp-1200910	0.005943	-0.57862	16

LiH2N	MP	mp-23702	0	-0.59054	4
Li2N*	MP	mp-1062345	0.263625	-0.17276	3
Li3N	HSC	-	-	-	-
Li3N**	MP	mp-2251	0	-0.4825	4
Li3N2*	MP	mp-1222421	0.759322	0.359824	5
LiN*	MP	mp-1059612	1.335792	0.99163	2
LiN3	MP	mp-2659	0	-0.20582	4

Table S8: The Mn-based system

Formula	**Source**	**mpid**	**E_hull [eV/atom]**	**E_form [eV/atom]**	**n**
Mn	HSC	-	-	-	-
Mn29H2*	MP	mp-1222194	0	-0.01634	31
MnH*	MP	mp-24416	0.150346	0.141612	2
Mn(H15N8)2*	MP	mp-1195097	0.009936	-0.36817	47
Mn(H2N)2*	MP	mp-703486	0.503855	0.08049	7
Mn2N	MP	mp-9981	0	-0.43548	3
Mn3N2	HSC	-	-	-	-
Mn3N4*	MP	mp-1080204	0.076293	-0.20366	7
Mn4N	HSC	-	-	-	-
Mn5N2	HSC	-	-	-	-
MnN	MP	mp-1009130	0.015086	-0.31153	2

Table S9: The Mo-based system

Formula	**Source**	**mpid**	**E_hull [eV/atom]**	**E_form [eV/atom]**	**n**
Mo	HSC	-	-	-	-
Mo2	HSC	-	-	-	-
Mo3H	MP	mp-975912	0.850179	0.850179	4
MoH	MP	mp-24417	0.393956	0.393956	2
Mo15N16*	MP	mp-530081	0	-0.53798	31
Mo2N	HSC	-	-	-	-
Mo2N**	MP	mp-27953	0.004064	-0.36008	3
Mo2N3*	MP	mp-1080195	0.155517	-0.28922	5
Mo3N2*	MP	mp-32652	0.571802	0.134825	5
MoN	HSC	-	-	-	-
MoN**	MP	mp-2811	0	-0.54622	2
MoN2	MP	mp-1402363	0.274727	-0.09588	3

Table S10: The Ni-based system

Formula	**Source**	**mpid**	**E_hull [eV/atom]**	**E_form [eV/atom]**	**n**
Ni	HSC	-	-	-	-
Ni2H	MP	mp-753890	0.046298	0.03888	3
Ni3H*	MP	mp-976948	0.515277	0.509713	4
NiH	MP	mp-24719	0	-0.01113	2
NiH0.5	HSC	-	-	-	-
NiH0.59	HSC	-	-	-	-
NiH0.68	HSC	-	-	-	-
NiH3*	MP	mp-973963	0.219315	0.213751	4
Ni(H2N)2*	MP	mp-28686	0.024374	-0.24142	7

Ni3N	HSC	-	-	-	-
Ni3N**	MP	mp-2033	0.014725	0.014725	4
Ni4N*	MP	mp-1094090	0.066688	0.066688	5
Ni4N3*	MP	mp-1094084	0.29447	0.29447	7
NiN	MP	mp-973933	0.31253	0.31253	2

Table S11: The Sr-based system

Formula	**Source**	**mpid**	**E_hull [eV/atom]**	**E_form [eV/atom]**	**n**
Sr	HSC	-	-	-	-
Sr3H*	MP	mp-1187129	0.68131	0.438468	4
SrH2	HSC	-	-	-	-
SrH2**	MP	mp-23714	0	-0.64758	3
SrH3	MP	mp-978856	0.340568	-0.14512	4
Sr(H2N)2*	MP	mp-643905	0	-0.65119	7
Sr2HN	MP	mp-690794	0	-0.75828	4
SrHN*	MP	mp-1187172	0	-0.82252	3
Sr2N	MP	mp-1245	0	-0.67197	3
Sr3N2	HSC	-	-	-	-
Sr3N2**	MP	mp-986716	0.03106	-0.63965	5
Sr4N3*	MP	mp-1173210	0.145913	-0.52426	7
SrN	MP	mp-29973	0	-0.66883	2
SrN2	MP	mp-10564	0	-0.62324	3
SrN6*	MP	mp-2131	0.009174	-0.25793	7

Table S12: The W-based system

Formula	**Source**	**mpid**	**E_hull [eV/atom]**	**E_form [eV/atom]**	**n**
W	HSC	-	-	-	-
W2N	HSC	-	-	-	-
W2N3*	MP	mp-1216242	0	-0.5573	5
W3N4	MP	mp-8102	0.365057	-0.16571	7
W7N6*	MP	mp-1216967	0.145784	-0.28291	13
WN	MP	mp-991	0.288264	-0.17616	2
WN18*	MP	mp-672264	0.304768	0.231438	19
WN2	MP	mp-2679804	0.063144	-0.40128	3
WN6*	MP	mp-1208477	2.410438	2.2114	7

Table S13: The Zn-based system

Formula	**Source**	**mpid**	**E_hull [eV/atom]**	**E_form [eV/atom]**	**n**
Zn	HSC	-	-	-	-
ZnH*		mp-971820	0.326733	0.326733	2
ZnH6*		mp-1207466	0.028949	0.028949	7
Zn(H15N8)2*		mp-1195558	0	-0.37232	47
Zn(H2N)2*		mp-24694	0	-0.41502	7
Zn(H4N5)2*		mp-1188715	0.12868	-0.14239	19
Zn3N*		mp-981366	0.769759	0.742932	4
Zn3N2	HSC	-	-	-	-
Zn3N2**		mp-9460	0	-0.04292	5
ZnN		mp-971911	0.555736	0.519967	2

ZnN6*		mp-1103897	0.089476	0.08187	7

1.4 Reactions

The following tables contain all reactions considered in the combined theoretical and experimental screenings. All possible combinations with the materials listed in Section 1.2 have been included. '*dm_stoich [%]'* is the stoichiometric weight change in % from the reactant solid to the product solid. *'h298 [kJ/mol]'* is the standard enthalpy change of the reaction at 25°C. *'T_eq [°C]'* is the equilibrium temperature. *'Type'* denotes if the reaction has an exergonic region, i.e. reaction proceeds spontaneously in the investigated temperature range 0-800°C.

Table S14: The Al-based system

ID	Reaction	dm_stoich [%]	h298 [kJ/mol]	T_eq [°C]	Type
Al-R01	6Al + H2 = 2Al3H	1.25	-	-	-
Al-R02	1/6Al + H2 = 1/6AlH12	44.83	-	-	-
Al-R03	2/3Al + H2 = 2/3AlH3	11.21	-7.6	-	endergonic
Al-R04	1/3Al + H2 = 1/3AlH6	22.41	-	-	-
Al-R05	2/35Al3H + H2 = 6/35AlH12	43.05	-	-	-
Al-R06	1/4Al3H + H2 = 3/4AlH3	9.84	-	-	-
Al-R07	2/17Al3H + H2 = 6/17AlH6	20.91	-	-	-
Al-R08	2/9AlH3 + H2 = 2/9AlH12	30.23	-	-	-
Al-R09	2/3AlH3 + H2 = 2/3AlH6	10.08	-	-	-
Al-R10	1/3AlH6 + H2 = 1/3AlH12	18.31	-	-	-
Al-R11	6AlN + H2 = 2Al3H + 3N2	-33.35	-	-	-
Al-R12	1/6AlN + H2 = 1/6AlH12 + 1/12N2	-4.66	-	-	-
Al-R13	2/3AlN + H2 = 2/3AlH3 + 1/3N2	-26.79	204.39	-	endergonic
Al-R14	1/3AlN + H2 = 1/3AlH6 + 1/6N2	-19.42	-	-	-
Al-R15	2/3AlN + H2 = 2/3Al + 2/3NH3	-34.17	181.39	-	endergonic
Al-R16	3/5AlN + H2 = 1/5Al3H + 3/5NH3	-33.35	-	-	-
Al-R17	2/15AlN + H2 = 2/15AlH12 + 2/15NH3	-4.66	-	-	-
Al-R18	1/3AlN + H2 = 1/3AlH3 + 1/3NH3	-26.79	86.9	-	endergonic
Al-R19	2/9AlN + H2 = 2/9AlH6 + 2/9NH3	-19.42	-	-	-
Al-R20	2Al + N2 = 2AlN	51.91	-635.97	-	exergonic
Al-R21	2/3Al3H + N2 = 2AlN + 1/3H2	50.04	-	-	-
Al-R22	6Al3H + N2 = 18Al + 2NH3	-1.23	-	-	-
Al-R23	3/5Al3H + N2 = 9/5AlN + 1/5NH3	50.04	-	-	-
Al-R24	2AlH12 + N2 = 2AlN + 12H2	4.89	-	-	-
Al-R25	1/2AlH12 + N2 = 1/2Al + 2NH3	-30.95	-	-	-
Al-R26	18/35AlH12 + N2 = 6/35Al3H + 2NH3	-30.09	-	-	-
Al-R27	2/3AlH12 + N2 = 2/3AlH3 + 2NH3	-23.22	-	-	-
Al-R28	AlH12 + N2 = AlH6 + 2NH3	-15.48	-	-	-
Al-R29	2/5AlH12 + N2 = 2/5AlN + 8/5NH3	4.89	-	-	-

Al-R30	2AlH3 + N2 = 2AlN + 3H2	36.6	-613.17	-	exergonic
Al-R31	2AlH3 + N2 = 2Al + 2NH3	-10.08	-69	-	exergonic
Al-R32	9/4AlH3 + N2 = 3/4Al3H + 2NH3	-8.96	-	-	-
Al-R33	AlH3 + N2 = AlN + NH3	36.6	-352.48	-	exergonic
Al-R34	2AlH6 + N2 = 2AlN + 6H2	24.1	-	-	-
Al-R35	AlH6 + N2 = Al + 2NH3	-18.31	-	-	-
Al-R36	18/17AlH6 + N2 = 6/17Al3H + 2NH3	-17.29	-	-	-
Al-R37	2AlH6 + N2 = 2AlH3 + 2NH3	-9.16	-	-	-
Al-R38	2/3AlH6 + N2 = 2/3AlN + 4/3NH3	24.1	-	-	-

Table S15: The Ca-based system

ID	Reaction	dm_stoich [%]	h298 [kJ/mol]	T_eq [°C]	Type
Ca-R001	Ca + H2 = CaH2	5.03	-176.98	-	exergonic
Ca-R002	2/3Ca + H2 = 2/3CaH3	7.55	-	-	-
Ca-R003	Ca(H2N)2 + H2 = Ca + 2NH3	-44.43	-	-	-
Ca-R004	1/2Ca(H2N)2 + H2 = 1/2CaH2 + NH3	-41.64	-	-	-
Ca-R005	2/5Ca(H2N)2 + H2 = 2/5CaH3 + 4/5NH3	-40.24	-	-	-
Ca-R006	32/9Ca(H2N)2 + H2 = 2/9Ca16HN8 + 16/3NH3	-34.63	-	-	-
Ca-R007	2Ca(H2N)2 + H2 = Ca2HN + 3NH3	-34.02	-	-	-
Ca-R008	16/7Ca(H2N)2 + H2 = 2/7Ca8H3N4 + 24/7NH3	-34.2	-	-	-
Ca-R009	4Ca(H2N)2 + H2 = 2Ca2N + 6NH3	-34.72	-	-	-
Ca-R010	1/11Ca11N8 + H2 = CaH2 + 4/11N2	-16.26	-	-	-
Ca-R011	2/33Ca11N8 + H2 = 2/3CaH3 + 8/33N2	-14.25	-	-	-
Ca-R012	32/11Ca11N8 + H2 = 2Ca16HN8 + 40/11N2	-6.21	-	-	-
Ca-R013	4/11Ca11N8 + H2 = 2Ca2HN + 5/11N2	-5.33	-	-	-
Ca-R014	16/33Ca11N8 + H2 = 2/3Ca8H3N4 + 20/33N2	-5.58	-	-	-
Ca-R015	1/12Ca11N8 + H2 = 11/12Ca + 2/3NH3	-20.27	-	-	-
Ca-R016	1/23Ca11N8 + H2 = 11/23CaH2 + 8/23NH3	-16.26	-	-	-
Ca-R017	2/57Ca11N8 + H2 = 22/57CaH3 + 16/57NH3	-14.25	-	-	-
Ca-R018	32/131Ca11N8 + H2 = 22/131Ca16HN8 + 80/131NH3	-6.21	-	-	-
Ca-R019	2/13Ca11N8 + H2 = 11/13Ca2HN + 5/13NH3	-5.33	-	-	-
Ca-R020	16/93Ca11N8 + H2 = 22/93Ca8H3N4 + 40/93NH3	-5.58	-	-	-
Ca-R021	4/15Ca11N8 + H2 = 22/15Ca2N + 2/3NH3	-6.33	-	-	-
Ca-R022	Ca11N8 + H2 = 11/3Ca3N2 + 2/3NH3	-1.69	-	-	-
Ca-R023	2/31Ca16HN8 + H2 = 32/31CaH2 + 8/31N2	-10.71	-	-	-
Ca-R024	2/47Ca16HN8 + H2 = 32/47CaH3 + 8/47N2	-8.57	-	-	-
Ca-R025	2/7Ca16HN8 + H2 = 16/7Ca2HN	0.94	-	-	-
Ca-R026	2/5Ca16HN8 + H2 = 4/5Ca8H3N4	0.67	-	-	-
Ca-R027	2/23Ca16HN8 + H2 = 32/23Ca + 16/23NH3	-14.99	-	-	-
Ca-R028	2/55Ca16HN8 + H2 = 32/55CaH2 + 16/55NH3	-10.71	-	-	-
Ca-R029	2/71Ca16HN8 + H2 = 32/71CaH3 + 16/71NH3	-8.57	-	-	-
Ca-R030	2/3Ca2HN + H2 = 4/3CaH2 + 1/3N2	-11.54	-	-	-
Ca-R031	2/5Ca2HN + H2 = 4/5CaH3 + 1/5N2	-9.42	-	-	-
Ca-R032	Ca2HN + H2 = 2Ca + NH3	-15.78	-	-	-
Ca-R033	1/3Ca2HN + H2 = 2/3CaH2 + 1/3NH3	-11.54	-	-	-

Ca-R034	1/4Ca2HN + H2 = 1/2CaH3 + 1/4NH3	-9.42	-	-	-
Ca-R035	1/2Ca2N + H2 = CaH2 + 1/4N2	-10.59	-47.06	235.2	exergonic
Ca-R036	1/3Ca2N + H2 = 2/3CaH3 + 1/6N2	-8.45	-	-	-
Ca-R037	16Ca2N + H2 = 2Ca16HN8	0.13	-	-	-
Ca-R038	2Ca2N + H2 = 2Ca2HN	1.07	-	-	-
Ca-R039	8/3Ca2N + H2 = 2/3Ca8H3N4	0.8	-	-	-
Ca-R040	2/3Ca2N + H2 = 4/3Ca + 2/3NH3	-14.88	142.63	-	endergonic
Ca-R041	2/7Ca2N + H2 = 4/7CaH2 + 2/7NH3	-10.59	-40	216.4	exergonic
Ca-R042	2/9Ca2N + H2 = 4/9CaH3 + 2/9NH3	-8.45	-	-	-
Ca-R043	1/3Ca3N2 + H2 = CaH2 + 1/3N2	-14.82	-33.31	259.7	exergonic
Ca-R044	2/9Ca3N2 + H2 = 2/3CaH3 + 2/9N2	-12.78	-	-	-
Ca-R045	32/3Ca3N2 + H2 = 2Ca16HN8 + 8/3N2	-4.6	-	-	-
Ca-R046	4/3Ca3N2 + H2 = 2Ca2HN + 1/3N2	-3.7	-	-	-
Ca-R047	16/9Ca3N2 + H2 = 2/3Ca8H3N4 + 4/9N2	-3.96	-	-	-
Ca-R048	1/3Ca3N2 + H2 = Ca + 2/3NH3	-18.9	113.07	-	endergonic
Ca-R049	1/6Ca3N2 + H2 = 1/2CaH2 + 1/3NH3	-14.82	-31.96	220.2	exergonic
Ca-R050	2/15Ca3N2 + H2 = 2/5CaH3 + 4/15NH3	-12.78	-	-	-
Ca-R051	32/27Ca3N2 + H2 = 2/9Ca16HN8 + 16/27NH3	-4.6	-	-	-
Ca-R052	2/3Ca3N2 + H2 = Ca2HN + 1/3NH3	-3.7	-	-	-
Ca-R053	16/21Ca3N2 + H2 = 2/7Ca8H3N4 + 8/21NH3	-3.96	-	-	-
Ca-R054	4/3Ca3N2 + H2 = 2Ca2N + 2/3NH3	-4.72	24.39	170.3	exergonic
Ca-R055	2/13Ca8H3N4 + H2 = 16/13CaH2 + 4/13N2	-11.31	-	-	-
Ca-R056	2/21Ca8H3N4 + H2 = 16/21CaH3 + 4/21N2	-9.18	-	-	-
Ca-R057	2Ca8H3N4 + H2 = 8Ca2HN	0.27	-	-	-
Ca-R058	2/9Ca8H3N4 + H2 = 16/9Ca + 8/9NH3	-15.55	-	-	-
Ca-R059	2/25Ca8H3N4 + H2 = 16/25CaH2 + 8/25NH3	-11.31	-	-	-
Ca-R060	2/33Ca8H3N4 + H2 = 16/33CaH3 + 8/33NH3	-9.18	-	-	-
Ca-R061	2CaH2 + H2 = 2CaH3	2.39	-	-	-
Ca-R062	2CaHN + H2 = 2CaH2 + N2	-23.59	-	-	-
Ca-R063	CaHN + H2 = CaH3 + 1/2N2	-21.77	-	-	-
Ca-R064	CaHN + H2 = Ca + NH3	-27.25	-	-	-
Ca-R065	1/2CaHN + H2 = 1/2CaH2 + 1/2NH3	-23.59	-	-	-
Ca-R066	2/5CaHN + H2 = 2/5CaH3 + 2/5NH3	-21.77	-	-	-
Ca-R067	32/9CaHN + H2 = 2/9Ca16HN8 + 16/9NH3	-14.43	-	-	-
Ca-R068	2CaHN + H2 = Ca2HN + NH3	-13.63	-	-	-
Ca-R069	16/7CaHN + H2 = 2/7Ca8H3N4 + 8/7NH3	-13.86	-	-	-
Ca-R070	4CaHN + H2 = 2Ca2N + 2NH3	-14.54	-	-	-
Ca-R071	CaN + H2 = CaH2 + 1/2N2	-22.17	-	-	-
Ca-R072	2/3CaN + H2 = 2/3CaH3 + 1/3N2	-20.31	-	-	-
Ca-R073	32CaN + H2 = 2Ca16HN8 + 8N2	-12.83	-	-	-
Ca-R074	4CaN + H2 = 2Ca2HN + N2	-12.02	-	-	-
Ca-R075	16/3CaN + H2 = 2/3Ca8H3N4 + 4/3N2	-12.25	-	-	-
Ca-R076	2CaN + H2 = 2CaHN	1.86	-	-	-
Ca-R077	2/3CaN + H2 = 2/3Ca + 2/3NH3	-25.9	-	-	-
Ca-R078	2/5CaN + H2 = 2/5CaH2 + 2/5NH3	-22.17	-	-	-
Ca-R079	1/3CaN + H2 = 1/3CaH3 + 1/3NH3	-20.31	-	-	-
Ca-R080	32/25CaN + H2 = 2/25Ca16HN8 + 16/25NH3	-12.83	-	-	-
Ca-R081	CaN + H2 = 1/2Ca2HN + 1/2NH3	-12.02	-	-	-
Ca-R082	16/15CaN + H2 = 2/15Ca8H3N4 + 8/15NH3	-12.25	-	-	-

Ca-R083	22/9CaN + H2 = 2/9Ca11N8 + 2/3NH3	-7.06	-	-	-
Ca-R084	4/3CaN + H2 = 2/3Ca2N + 2/3NH3	-12.95	-	-	-
Ca-R085	2CaN + H2 = 2/3Ca3N2 + 2/3NH3	-8.63	-	-	-
Ca-R086	CaN2 + H2 = CaH2 + N2	-38.18	8.05	-	exergonic
Ca-R087	2/3CaN2 + H2 = 2/3CaH3 + 2/3N2	-36.7	-	-	-
Ca-R088	1/2CaN2 + H2 = 1/2Ca(H2N)2	5.92	-	-	-
Ca-R089	32CaN2 + H2 = 2Ca16HN8 + 24N2	-30.76	-	-	-
Ca-R090	4CaN2 + H2 = 2Ca2HN + 3N2	-30.12	-	-	-
Ca-R091	16/3CaN2 + H2 = 2/3Ca8H3N4 + 4N2	-30.3	-	-	-
Ca-R092	2CaN2 + H2 = 2CaHN + N2	-19.09	-	-	-
Ca-R093	1/3CaN2 + H2 = 1/3Ca + 2/3NH3	-41.14	31.08	-	endergonic
Ca-R094	1/4CaN2 + H2 = 1/4CaH2 + 1/2NH3	-38.18	-20.94	228.3	exergonic
Ca-R095	2/9CaN2 + H2 = 2/9CaH3 + 4/9NH3	-36.7	-	-	-
Ca-R096	32/73CaN2 + H2 = 2/73Ca16HN8 + 48/73NH3	-30.76	-	-	-
Ca-R097	2/5CaN2 + H2 = 1/5Ca2HN + 3/5NH3	-30.12	-	-	-
Ca-R098	16/39CaN2 + H2 = 2/39Ca8H3N4 + 8/13NH3	-30.3	-	-	-
Ca-R099	1/2CaN2 + H2 = 1/2CaHN + 1/2NH3	-19.09	-	-	-
Ca-R100	11/21CaN2 + H2 = 1/21Ca11N8 + 2/3NH3	-26.18	-	-	-
Ca-R101	4/9CaN2 + H2 = 2/9Ca2N + 2/3NH3	-30.86	-6.1	271.8	exergonic
Ca-R102	1/2CaN2 + H2 = 1/6Ca3N2 + 2/3NH3	-27.43	-9.92	250.3	exergonic
Ca-R103	2/3CaN2 + H2 = 2/3CaN + 2/3NH3	-20.57	-	-	-
Ca-R104	CaN6 + H2 = CaH2 + 3N2	-66.09	-19.39	-	exergonic
Ca-R105	2/3CaN6 + H2 = 2/3CaH3 + 2N2	-65.27	-	-	-
Ca-R106	1/2CaN6 + H2 = 1/2Ca(H2N)2 + N2	-41.89	-	-	-
Ca-R107	32CaN6 + H2 = 2Ca16HN8 + 88N2	-62.02	-	-	-
Ca-R108	4CaN6 + H2 = 2Ca2HN + 11N2	-61.66	-	-	-
Ca-R109	16/3CaN6 + H2 = 2/3Ca8H3N4 + 44/3N2	-61.76	-	-	-
Ca-R110	2CaN6 + H2 = 2CaHN + 5N2	-55.61	-	-	-
Ca-R111	1/9CaN6 + H2 = 1/9Ca + 2/3NH3	-67.71	-13.09	367.6	exergonic
Ca-R112	1/10CaN6 + H2 = 1/10CaH2 + 3/5NH3	-66.09	-29.48	583.8	exergonic
Ca-R113	2/21CaN6 + H2 = 2/21CaH3 + 4/7NH3	-65.27	-	-	-
Ca-R114	1/8CaN6 + H2 = 1/8Ca(H2N)2 + 1/2NH3	-41.89	-	-	-
Ca-R115	32/265CaN6 + H2 = 2/265Ca16HN8 + 176/265NH3	-62.02	-	-	-
Ca-R116	2/17CaN6 + H2 = 1/17Ca2HN + 11/17NH3	-61.66	-	-	-
Ca-R117	16/135CaN6 + H2 = 2/135Ca8H3N4 + 88/135NH3	-61.76	-	-	-
Ca-R118	1/8CaN6 + H2 = 1/8CaHN + 5/8NH3	-55.61	-	-	-
Ca-R119	11/87CaN6 + H2 = 1/87Ca11N8 + 2/3NH3	-59.5	-	-	-
Ca-R120	4/33CaN6 + H2 = 2/33Ca2N + 2/3NH3	-62.07	-27.24	783	exergonic
Ca-R121	1/8CaN6 + H2 = 1/24Ca3N2 + 2/3NH3	-60.19	-28.86	767.3	exergonic
Ca-R122	2/15CaN6 + H2 = 2/15CaN + 2/3NH3	-56.43	-	-	-
Ca-R123	1/6CaN6 + H2 = 1/6CaN2 + 2/3NH3	-45.14	-35.17	-	exergonic
Ca-R124	11/4Ca + N2 = 1/4Ca11N8	25.42	-	-	-
Ca-R125	4Ca + N2 = 2Ca2N	17.47	-519.68	-	exergonic
Ca-R126	3Ca + N2 = Ca3N2	23.3	-431	-	exergonic
Ca-R127	2Ca + N2 = 2CaN	34.95	-	-	-
Ca-R128	Ca + N2 = CaN2	69.9	-185.03	-	exergonic
Ca-R129	1/3Ca + N2 = 1/3CaN6	209.7	-52.53	78.6	exergonic
Ca-R130	1/2Ca(H2N)2 + N2 = 1/2CaN6 + H2	72.09	-	-	-
Ca-R131	33Ca(H2N)2 + N2 = 3Ca11N8 + 44NH3	-30.31	-	-	-

Ca-R132	6Ca(H2N)2 + N2 = 6CaN + 8NH3	-25.01	-	-	-
Ca-R133	3/2Ca(H2N)2 + N2 = 3/2CaN2 + 2NH3	-5.59	-	-	-
Ca-R134	3/8Ca(H2N)2 + N2 = 3/8CaN6 + 1/2NH3	72.09	-	-	-
Ca-R135	2/3Ca11N8 + N2 = 22/3CaN	7.6	-	-	-
Ca-R136	1/7Ca11N8 + N2 = 11/7CaN2	35.47	-	-	-
Ca-R137	1/29Ca11N8 + N2 = 11/29CaN6	146.93	-	-	-
Ca-R138	11/20Ca16HN8 + N2 = 4/5Ca11N8 + 11/40H2	6.62	-	-	-
Ca-R139	3/4Ca16HN8 + N2 = 4Ca3N2 + 3/8H2	4.82	-	-	-
Ca-R140	1/4Ca16HN8 + N2 = 4CaN + 1/8H2	14.72	-	-	-
Ca-R141	1/12Ca16HN8 + N2 = 4/3CaN2 + 1/24H2	44.43	-	-	-
Ca-R142	1/44Ca16HN8 + N2 = 4/11CaN6 + 1/88H2	163.28	-	-	-
Ca-R143	66/131Ca16HN8 + N2 = 96/131Ca11N8 + 22/131NH3	6.62	-	-	-
Ca-R144	6Ca16HN8 + N2 = 48Ca2N + 2NH3	-0.13	-	-	-
Ca-R145	2/3Ca16HN8 + N2 = 32/9Ca3N2 + 2/9NH3	4.82	-	-	-
Ca-R146	6/25Ca16HN8 + N2 = 96/25CaN + 2/25NH3	14.72	-	-	-
Ca-R147	6/73Ca16HN8 + N2 = 96/73CaN2 + 2/73NH3	44.43	-	-	-
Ca-R148	6/265Ca16HN8 + N2 = 96/265CaN6 + 2/265NH3	163.28	-	-	-
Ca-R149	22/5Ca2HN + N2 = 4/5Ca11N8 + 11/5H2	5.63	-	-	-
Ca-R150	6Ca2HN + N2 = 4Ca3N2 + 3H2	3.85	-	-	-
Ca-R151	2Ca2HN + N2 = 4CaN + H2	13.66	-	-	-
Ca-R152	2/3Ca2HN + N2 = 4/3CaN2 + 1/3H2	43.09	-	-	-
Ca-R153	2/11Ca2HN + N2 = 4/11CaN6 + 1/11H2	160.84	-	-	-
Ca-R154	48/7Ca2HN + N2 = 6/7Ca16HN8 + 2NH3	-0.93	-	-	-
Ca-R155	24Ca2HN + N2 = 6Ca8H3N4 + 2NH3	-0.26	-	-	-
Ca-R156	33/13Ca2HN + N2 = 6/13Ca11N8 + 11/13NH3	5.63	-	-	-
Ca-R157	6Ca2HN + N2 = 6Ca2N + 2NH3	-1.06	-	-	-
Ca-R158	3Ca2HN + N2 = 2Ca3N2 + NH3	3.85	-	-	-
Ca-R159	3/2Ca2HN + N2 = 3CaN + 1/2NH3	13.66	-	-	-
Ca-R160	3/5Ca2HN + N2 = 6/5CaN2 + 1/5NH3	43.09	-	-	-
Ca-R161	3/17Ca2HN + N2 = 6/17CaN6 + 1/17NH3	160.84	-	-	-
Ca-R162	22/5Ca2N + N2 = 4/5Ca11N8	6.76	-	-	-
Ca-R163	6Ca2N + N2 = 4Ca3N2	4.96	-164.95	177.7	exergonic
Ca-R164	2Ca2N + N2 = 4CaN	14.88	-	-	-
Ca-R165	2/3Ca2N + N2 = 4/3CaN2	44.63	-73.48	154.4	exergonic
Ca-R166	2/11Ca2N + N2 = 4/11CaN6	163.63	-10.06	-	endergonic
Ca-R167	11Ca3N2 + N2 = 3Ca11N8	1.72	-	-	-
Ca-R168	2Ca3N2 + N2 = 6CaN	9.45	-	-	-
Ca-R169	1/2Ca3N2 + N2 = 3/2CaN2	37.79	-62.05	147.1	exergonic
Ca-R170	1/8Ca3N2 + N2 = 3/8CaN6	151.17	-5.22	-	endergonic
Ca-R171	11/10Ca8H3N4 + N2 = 4/5Ca11N8 + 33/20H2	5.91	-	-	-
Ca-R172	3/2Ca8H3N4 + N2 = 4Ca3N2 + 9/4H2	4.12	-	-	-
Ca-R173	1/2Ca8H3N4 + N2 = 4CaN + 3/4H2	13.96	-	-	-
Ca-R174	1/6Ca8H3N4 + N2 = 4/3CaN2 + 1/4H2	43.47	-	-	-
Ca-R175	1/22Ca8H3N4 + N2 = 4/11CaN6 + 3/44H2	161.53	-	-	-
Ca-R176	12/5Ca8H3N4 + N2 = 6/5Ca16HN8 + 2NH3	-0.66	-	-	-
Ca-R177	22/31Ca8H3N4 + N2 = 16/31Ca11N8 + 22/31NH3	5.91	-	-	-
Ca-R178	2Ca8H3N4 + N2 = 8Ca2N + 2NH3	-0.8	-	-	-
Ca-R179	6/7Ca8H3N4 + N2 = 16/7Ca3N2 + 6/7NH3	4.12	-	-	-
Ca-R180	2/5Ca8H3N4 + N2 = 16/5CaN + 2/5NH3	13.96	-	-	-

Ca-R181	2/13Ca8H3N4 + N2 = 16/13CaN2 + 2/13NH3	43.47	-	-	-
Ca-R182	2/45Ca8H3N4 + N2 = 16/45CaN6 + 2/45NH3	161.53	-	-	-
Ca-R183	4CaH2 + N2 = 1/4Ca16HN8 + 31/8H2	12	-	-	-
Ca-R184	4CaH2 + N2 = 2Ca2HN + 3H2	13.05	-	-	-
Ca-R185	4CaH2 + N2 = 1/2Ca8H3N4 + 13/4H2	12.75	-	-	-
Ca-R186	2CaH2 + N2 = 2CaHN + H2	30.88	-	-	-
Ca-R187	11/4CaH2 + N2 = 1/4Ca11N8 + 11/4H2	19.41	-	-	-
Ca-R188	4CaH2 + N2 = 2Ca2N + 4H2	11.85	188.24	235.2	exergonic
Ca-R189	3CaH2 + N2 = Ca3N2 + 3H2	17.39	99.94	259.7	exergonic
Ca-R190	2CaH2 + N2 = 2CaN + 2H2	28.49	-	-	-
Ca-R191	CaH2 + N2 = CaN2 + H2	61.76	-8.05	-	endergonic
Ca-R192	1/3CaH2 + N2 = 1/3CaN6 + 1/3H2	194.86	6.46	-	endergonic
Ca-R193	3CaH2 + N2 = 3Ca + 2NH3	-4.79	439.15	-	endergonic
Ca-R194	96/55CaH2 + N2 = 6/55Ca16HN8 + 62/55NH3	12	-	-	-
Ca-R195	2CaH2 + N2 = Ca2HN + NH3	13.05	-	-	-
Ca-R196	48/25CaH2 + N2 = 6/25Ca8H3N4 + 26/25NH3	12.75	-	-	-
Ca-R197	3/2CaH2 + N2 = 3/2CaHN + 1/2NH3	30.88	-	-	-
Ca-R198	33/23CaH2 + N2 = 3/23Ca11N8 + 22/23NH3	19.41	-	-	-
Ca-R199	12/7CaH2 + N2 = 6/7Ca2N + 8/7NH3	11.85	28.22	389.3	exergonic
Ca-R200	3/2CaH2 + N2 = 1/2Ca3N2 + NH3	17.39	4.08	-	endergonic
Ca-R201	6/5CaH2 + N2 = 6/5CaN + 4/5NH3	28.49	-	-	-
Ca-R202	3/4CaH2 + N2 = 3/4CaN2 + 1/2NH3	61.76	-28.99	97.1	exergonic
Ca-R203	3/10CaH2 + N2 = 3/10CaN6 + 1/5NH3	194.86	-3.36	-	endergonic
Ca-R204	4CaH3 + N2 = 1/4Ca16HN8 + 47/8H2	9.38	-	-	-
Ca-R205	4CaH3 + N2 = 2Ca2HN + 5H2	10.4	-	-	-
Ca-R206	4CaH3 + N2 = 1/2Ca8H3N4 + 21/4H2	10.11	-	-	-
Ca-R207	2CaH3 + N2 = 2CaHN + 2H2	27.82	-	-	-
Ca-R208	11/4CaH3 + N2 = 1/4Ca11N8 + 33/8H2	16.62	-	-	-
Ca-R209	4CaH3 + N2 = 2Ca2N + 6H2	9.23	-	-	-
Ca-R210	3CaH3 + N2 = Ca3N2 + 9/2H2	14.65	-	-	-
Ca-R211	2CaH3 + N2 = 2CaN + 3H2	25.48	-	-	-
Ca-R212	CaH3 + N2 = CaN2 + 3/2H2	57.98	-	-	-
Ca-R213	1/3CaH3 + N2 = 1/3CaN6 + 1/2H2	187.97	-	-	-
Ca-R214	2CaH3 + N2 = 2Ca + 2NH3	-7.02	-	-	-
Ca-R215	6CaH3 + N2 = 6CaH2 + 2NH3	-2.34	-	-	-
Ca-R216	96/71CaH3 + N2 = 6/71Ca16HN8 + 94/71NH3	9.38	-	-	-
Ca-R217	3/2CaH3 + N2 = 3/4Ca2HN + 5/4NH3	10.4	-	-	-
Ca-R218	16/11CaH3 + N2 = 2/11Ca8H3N4 + 14/11NH3	10.11	-	-	-
Ca-R219	6/5CaH3 + N2 = 6/5CaHN + 4/5NH3	27.82	-	-	-
Ca-R220	22/19CaH3 + N2 = 2/19Ca11N8 + 22/19NH3	16.62	-	-	-
Ca-R221	4/3CaH3 + N2 = 2/3Ca2N + 4/3NH3	9.23	-	-	-
Ca-R222	6/5CaH3 + N2 = 2/5Ca3N2 + 6/5NH3	14.65	-	-	-
Ca-R223	CaH3 + N2 = CaN + NH3	25.48	-	-	-
Ca-R224	2/3CaH3 + N2 = 2/3CaN2 + 2/3NH3	57.98	-	-	-
Ca-R225	2/7CaH3 + N2 = 2/7CaN6 + 2/7NH3	187.97	-	-	-
Ca-R226	2CaHN + N2 = 2CaN2 + H2	23.59	-	-	-
Ca-R227	2/5CaHN + N2 = 2/5CaN6 + 1/5H2	125.29	-	-	-
Ca-R228	33CaHN + N2 = 3Ca11N8 + 11NH3	-8.76	-	-	-
Ca-R229	6CaHN + N2 = 6CaN + 2NH3	-1.83	-	-	-

Ca-R230	3/2CaHN + N2 = 3/2CaN2 + 1/2NH3	23.59	-	-	-
Ca-R231	3/8CaHN + N2 = 3/8CaN6 + 1/8NH3	125.29	-	-	-
Ca-R232	2CaN + N2 = 2CaN2	25.9	-	-	-
Ca-R233	2/5CaN + N2 = 2/5CaN6	129.49	-	-	-
Ca-R234	1/2CaN2 + N2 = 1/2CaN6	82.28	13.72	-	endergonic

Table S16: The Co-based system

ID	Reaction	dm_stoich [%]	h298 [kJ/mol]	T_eq [°C]	Type
Co-R001	6Co + H2 = 2Co3H	0.57	-16.75	-	endergonic
Co-R002	8Co + H2 = 2Co4H	0.43	-	-	-
Co-R003	2Co + H2 = 2CoH	1.71	-	-	-
Co-R004	2/3Co + H2 = 2/3CoH3	5.13	-	-	-
Co-R005	3Co2N + H2 = 2Co3H + 3/2N2	-10.11	-171.23	-	exergonic
Co-R006	4Co2N + H2 = 2Co4H + 2N2	-10.24	-	-	-
Co-R007	Co2N + H2 = 2CoH + 1/2N2	-9.09	-	-	-
Co-R008	1/3Co2N + H2 = 2/3CoH3 + 1/6N2	-6.04	-	-	-
Co-R009	2/3Co2N + H2 = 4/3Co + 2/3NH3	-10.62	-64.93	-	exergonic
Co-R010	6/11Co2N + H2 = 4/11Co3H + 6/11NH3	-10.11	-56.17	-	exergonic
Co-R011	4/7Co2N + H2 = 2/7Co4H + 4/7NH3	-10.24	-	-	-
Co-R012	2/5Co2N + H2 = 4/5CoH + 2/5NH3	-9.09	-	-	-
Co-R013	2/9Co2N + H2 = 4/9CoH3 + 2/9NH3	-6.04	-	-	-
Co-R014	2Co2N + H2 = 4/3Co3N + 2/3NH3	-3.54	-122.43	-	exergonic
Co-R015	4/3Co2N + H2 = 2/3Co4N + 2/3NH3	-5.31	-	-	-
Co-R016	Co3H + H2 = 3CoH	1.13	-	-	-
Co-R017	1/4Co3H + H2 = 3/4CoH3	4.54	-	-	-
Co-R018	2Co3N + H2 = 2Co3H + N2	-6.81	-33.49	-	exergonic
Co-R019	8/3Co3N + H2 = 2Co4H + 4/3N2	-6.94	-	-	-
Co-R020	2/3Co3N + H2 = 2CoH + 1/3N2	-5.76	-	-	-
Co-R021	2/9Co3N + H2 = 2/3CoH3 + 1/9N2	-2.59	-	-	-
Co-R022	2/3Co3N + H2 = 2Co + 2/3NH3	-7.34	-36.18	-	exergonic
Co-R023	1/2Co3N + H2 = 1/2Co3H + 1/2NH3	-6.81	-31.32	352.1	exergonic
Co-R024	8/15Co3N + H2 = 2/5Co4H + 8/15NH3	-6.94	-	-	-
Co-R025	1/3Co3N + H2 = CoH + 1/3NH3	-5.76	-	-	-
Co-R026	1/6Co3N + H2 = 1/2CoH3 + 1/6NH3	-2.59	-	-	-
Co-R027	8/3Co3N + H2 = 2Co4N + 2/3NH3	-1.84	-	-	-
Co-R028	6Co4H + H2 = 8Co3H	0.14	-	-	-
Co-R029	2/3Co4H + H2 = 8/3CoH	1.28	-	-	-
Co-R030	2/11Co4H + H2 = 8/11CoH3	4.68	-	-	-
Co-R031	3/2Co4N + H2 = 2Co3H + 3/4N2	-5.07	-	-	-
Co-R032	2Co4N + H2 = 2Co4H + N2	-5.21	-	-	-
Co-R033	1/2Co4N + H2 = 2CoH + 1/4N2	-3.99	-	-	-
Co-R034	1/6Co4N + H2 = 2/3CoH3 + 1/12N2	-0.77	-	-	-
Co-R035	2/3Co4N + H2 = 8/3Co + 2/3NH3	-5.61	-	-	-
Co-R036	6/13Co4N + H2 = 8/13Co3H + 6/13NH3	-5.07	-	-	-
Co-R037	1/2Co4N + H2 = 1/2Co4H + 1/2NH3	-5.21	-	-	-
Co-R038	2/7Co4N + H2 = 8/7CoH + 2/7NH3	-3.99	-	-	-
Co-R039	2/15Co4N + H2 = 8/15CoH3 + 2/15NH3	-0.77	-	-	-
Co-R040	CoH + H2 = CoH3	3.36	-	-	-

Co-R041	6CoN + H2 = 2Co3H + 3N2	-18.74	-135.88	-	exergonic
Co-R042	8CoN + H2 = 2Co4H + 4N2	-18.86	-	-	-
Co-R043	2CoN + H2 = 2CoH + N2	-17.82	-	-	-
Co-R044	2/3CoN + H2 = 2/3CoH3 + 1/3N2	-15.06	-	-	-
Co-R045	2/3CoN + H2 = 2/3Co + 2/3NH3	-19.2	-43.83	-	exergonic
Co-R046	3/5CoN + H2 = 1/5Co3H + 3/5NH3	-18.74	-41.13	798.6	exergonic
Co-R047	8/13CoN + H2 = 2/13Co4H + 8/13NH3	-18.86	-	-	-
Co-R048	1/2CoN + H2 = 1/2CoH + 1/2NH3	-17.82	-	-	-
Co-R049	1/3CoN + H2 = 1/3CoH3 + 1/3NH3	-15.06	-	-	-
Co-R050	4/3CoN + H2 = 2/3Co2N + 2/3NH3	-9.6	-22.74	422.8	exergonic
Co-R051	CoN + H2 = 1/3Co3N + 2/3NH3	-12.8	-47.66	-	exergonic
Co-R052	8/9CoN + H2 = 2/9Co4N + 2/3NH3	-14.4	-	-	-
Co-R053	6CoN12 + H2 = 2Co3H + 36N2	-73.89	-	-	-
Co-R054	8CoN12 + H2 = 2Co4H + 48N2	-73.93	-	-	-
Co-R055	2CoN12 + H2 = 2CoH + 12N2	-73.6	-	-	-
Co-R056	2/3CoN12 + H2 = 2/3CoH3 + 4N2	-72.71	-	-	-
Co-R057	1/18CoN12 + H2 = 1/18Co + 2/3NH3	-74.04	-	-	-
Co-R058	6/109CoN12 + H2 = 2/109Co3H + 72/109NH3	-73.89	-	-	-
Co-R059	8/145CoN12 + H2 = 2/145Co4H + 96/145NH3	-73.93	-	-	-
Co-R060	2/37CoN12 + H2 = 2/37CoH + 24/37NH3	-73.6	-	-	-
Co-R061	2/39CoN12 + H2 = 2/39CoH3 + 8/13NH3	-72.71	-	-	-
Co-R062	4/69CoN12 + H2 = 2/69Co2N + 2/3NH3	-70.96	-	-	-
Co-R063	2/35CoN12 + H2 = 2/105Co3N + 2/3NH3	-71.98	-	-	-
Co-R064	8/141CoN12 + H2 = 2/141Co4N + 2/3NH3	-72.5	-	-	-
Co-R065	2/33CoN12 + H2 = 2/33CoN + 2/3NH3	-67.87	-	-	-
Co-R066	2/27CoN12 + H2 = 2/27CoN3 + 2/3NH3	-55.53	-	-	-
Co-R067	6CoN3 + H2 = 2Co3H + 9N2	-41.29	-	-	-
Co-R068	8CoN3 + H2 = 2Co4H + 12N2	-41.37	-	-	-
Co-R069	2CoN3 + H2 = 2CoH + 3N2	-40.63	-	-	-
Co-R070	2/3CoN3 + H2 = 2/3CoH3 + N2	-38.63	-	-	-
Co-R071	2/9CoN3 + H2 = 2/9Co + 2/3NH3	-41.62	-	-	-
Co-R072	3/14CoN3 + H2 = 1/14Co3H + 9/14NH3	-41.29	-	-	-
Co-R073	8/37CoN3 + H2 = 2/37Co4H + 24/37NH3	-41.37	-	-	-
Co-R074	1/5CoN3 + H2 = 1/5CoH + 3/5NH3	-40.63	-	-	-
Co-R075	1/6CoN3 + H2 = 1/6CoH3 + 1/2NH3	-38.63	-	-	-
Co-R076	4/15CoN3 + H2 = 2/15Co2N + 2/3NH3	-34.69	-	-	-
Co-R077	1/4CoN3 + H2 = 1/12Co3N + 2/3NH3	-37	-	-	-
Co-R078	8/33CoN3 + H2 = 2/33Co4N + 2/3NH3	-38.16	-	-	-
Co-R079	1/3CoN3 + H2 = 1/3CoN + 2/3NH3	-27.75	-	-	-
Co-R080	4Co + N2 = 2Co2N	11.88	102.99	-	endergonic
Co-R081	6Co + N2 = 2Co3N	7.92	16.74	-	endergonic
Co-R082	8Co + N2 = 2Co4N	5.94	-	-	-
Co-R083	2Co + N2 = 2CoN	23.77	39.71	-	endergonic
Co-R084	1/6Co + N2 = 1/6CoN12	285.21	-	-	-
Co-R085	2/3Co + N2 = 2/3CoN3	71.3	-	-	-
Co-R086	2Co2N + N2 = 4CoN	10.62	-23.57	-	endergonic
Co-R087	2/23Co2N + N2 = 4/23CoN12	244.3	-	-	-
Co-R088	2/5Co2N + N2 = 4/5CoN3	53.11	-	-	-
Co-R089	4/3Co3H + N2 = 2Co2N + 2/3H2	11.25	114.16	-	endergonic

Co-R090	2Co3H + N2 = 2Co3N + H2	7.31	33.49	-	endergonic
Co-R091	8/3Co3H + N2 = 2Co4N + 4/3H2	5.34	-	-	-
Co-R092	2/3Co3H + N2 = 2CoN + 1/3H2	23.07	45.29	-	endergonic
Co-R093	1/18Co3H + N2 = 1/6CoN12 + 1/36H2	283.03	-	-	-
Co-R094	2/9Co3H + N2 = 2/3CoN3 + 1/9H2	70.33	-	-	-
Co-R095	6Co3H + N2 = 18Co + 2NH3	-0.57	-41.54	-	exergonic
Co-R096	24Co3H + N2 = 18Co4H + 2NH3	-0.14	-	-	-
Co-R097	12/11Co3H + N2 = 18/11Co2N + 4/11NH3	11.25	76.71	-	endergonic
Co-R098	3/2Co3H + N2 = 3/2Co3N + 1/2NH3	7.31	2.17	-	endergonic
Co-R099	24/13Co3H + N2 = 18/13Co4N + 8/13NH3	5.34	-	-	-
Co-R100	3/5Co3H + N2 = 9/5CoN + 1/5NH3	23.07	31.59	-	endergonic
Co-R101	6/109Co3H + N2 = 18/109CoN12 + 2/109NH3	283.03	-	-	-
Co-R102	3/14Co3H + N2 = 9/14CoN3 + 1/14NH3	70.33	-	-	-
Co-R103	4Co3N + N2 = 6Co2N	3.67	275.49	-	endergonic
Co-R104	Co3N + N2 = 3CoN	14.68	51.2	-	endergonic
Co-R105	2/35Co3N + N2 = 6/35CoN12	256.93	-	-	-
Co-R106	1/4Co3N + N2 = 3/4CoN3	58.73	-	-	-
Co-R107	Co4H + N2 = 2Co2N + 1/2H2	11.41	-	-	-
Co-R108	3/2Co4H + N2 = 2Co3N + 3/4H2	7.46	-	-	-
Co-R109	2Co4H + N2 = 2Co4N + H2	5.49	-	-	-
Co-R110	1/2Co4H + N2 = 2CoN + 1/4H2	23.24	-	-	-
Co-R111	1/24Co4H + N2 = 1/6CoN12 + 1/48H2	283.57	-	-	-
Co-R112	1/6Co4H + N2 = 2/3CoN3 + 1/12H2	70.57	-	-	-
Co-R113	6Co4H + N2 = 24Co + 2NH3	-0.43	-	-	-
Co-R114	6/7Co4H + N2 = 12/7Co2N + 2/7NH3	11.41	-	-	-
Co-R115	6/5Co4H + N2 = 8/5Co3N + 2/5NH3	7.46	-	-	-
Co-R116	3/2Co4H + N2 = 3/2Co4N + 1/2NH3	5.49	-	-	-
Co-R117	6/13Co4H + N2 = 24/13CoN + 2/13NH3	23.24	-	-	-
Co-R118	6/145Co4H + N2 = 24/145CoN12 + 2/145NH3	283.57	-	-	-
Co-R119	6/37Co4H + N2 = 24/37CoN3 + 2/37NH3	70.57	-	-	-
Co-R120	2Co4N + N2 = 4Co2N	5.61	-	-	-
Co-R121	6Co4N + N2 = 8Co3N	1.87	-	-	-
Co-R122	2/3Co4N + N2 = 8/3CoN	16.83	-	-	-
Co-R123	2/47Co4N + N2 = 8/47CoN12	263.61	-	-	-
Co-R124	2/11Co4N + N2 = 8/11CoN3	61.7	-	-	-
Co-R125	4CoH + N2 = 2Co2N + 2H2	10	-	-	-
Co-R126	6CoH + N2 = 2Co3N + 3H2	6.11	-	-	-
Co-R127	8CoH + N2 = 2Co4N + 4H2	4.16	-	-	-
Co-R128	2CoH + N2 = 2CoN + H2	21.69	-	-	-
Co-R129	1/6CoH + N2 = 1/6CoN12 + 1/12H2	278.73	-	-	-
Co-R130	2/3CoH + N2 = 2/3CoN3 + 1/3H2	68.42	-	-	-
Co-R131	6CoH + N2 = 6Co + 2NH3	-1.68	-	-	-
Co-R132	9CoH + N2 = 3Co3H + 2NH3	-1.12	-	-	-
Co-R133	8CoH + N2 = 2Co4H + 2NH3	-1.26	-	-	-
Co-R134	12/5CoH + N2 = 6/5Co2N + 4/5NH3	10	-	-	-
Co-R135	3CoH + N2 = Co3N + NH3	6.11	-	-	-
Co-R136	24/7CoH + N2 = 6/7Co4N + 8/7NH3	4.16	-	-	-
Co-R137	3/2CoH + N2 = 3/2CoN + 1/2NH3	21.69	-	-	-
Co-R138	6/37CoH + N2 = 6/37CoN12 + 2/37NH3	278.73	-	-	-

Co-R139	3/5CoH + N2 = 3/5CoN3 + 1/5NH3	68.42	-	-	-
Co-R140	4CoH3 + N2 = 2Co2N + 6H2	6.42	-	-	-
Co-R141	6CoH3 + N2 = 2Co3N + 9H2	2.66	-	-	-
Co-R142	8CoH3 + N2 = 2Co4N + 12H2	0.77	-	-	-
Co-R143	2CoH3 + N2 = 2CoN + 3H2	17.73	-	-	-
Co-R144	1/6CoH3 + N2 = 1/6CoN12 + 1/4H2	266.41	-	-	-
Co-R145	2/3CoH3 + N2 = 2/3CoN3 + H2	62.94	-	-	-
Co-R146	2CoH3 + N2 = 2Co + 2NH3	-4.88	-	-	-
Co-R147	9/4CoH3 + N2 = 3/4Co3H + 2NH3	-4.34	-	-	-
Co-R148	24/11CoH3 + N2 = 6/11Co4H + 2NH3	-4.47	-	-	-
Co-R149	3CoH3 + N2 = 3CoH + 2NH3	-3.25	-	-	-
Co-R150	4/3CoH3 + N2 = 2/3Co2N + 4/3NH3	6.42	-	-	-
Co-R151	3/2CoH3 + N2 = 1/2Co3N + 3/2NH3	2.66	-	-	-
Co-R152	8/5CoH3 + N2 = 2/5Co4N + 8/5NH3	0.77	-	-	-
Co-R153	CoH3 + N2 = CoN + NH3	17.73	-	-	-
Co-R154	2/13CoH3 + N2 = 2/13CoN12 + 2/13NH3	266.41	-	-	-
Co-R155	1/2CoH3 + N2 = 1/2CoN3 + 1/2NH3	62.94	-	-	-
Co-R156	2/11CoN + N2 = 2/11CoN12	211.24	-	-	-
Co-R157	CoN + N2 = CoN3	38.41	-	-	-
Co-R158	2/9CoN3 + N2 = 2/9CoN12	124.87	-	-	-

Table S17: The Cr-based system

ID	**Reaction**	**dm_stoich [%]**	**h298 [kJ/mol]**	**T_eq [°C]**	**Type**
Cr-R001	6Cr + H2 = 2Cr3H	0.65	-	-	-
Cr-R002	2Cr + H2 = 2CrH	1.94	64.04	-	endergonic
Cr-R003	Cr + H2 = CrH2	3.88	-	-	-
Cr-R004	2/3Cr + H2 = 2/3CrH3	5.82	-	-	-
Cr-R005	3Cr2N + H2 = 2Cr3H + 3/2N2	-11.3	-	-	-
Cr-R006	Cr2N + H2 = 2CrH + 1/2N2	-10.16	189.56	-	endergonic
Cr-R007	1/2Cr2N + H2 = CrH2 + 1/4N2	-8.45	-	-	-
Cr-R008	1/3Cr2N + H2 = 2/3CrH3 + 1/6N2	-6.74	-	-	-
Cr-R009	2/3Cr2N + H2 = 4/3Cr + 2/3NH3	-11.87	53.08	-	endergonic
Cr-R010	6/11Cr2N + H2 = 4/11Cr3H + 6/11NH3	-11.3	-	-	-
Cr-R011	2/5Cr2N + H2 = 4/5CrH + 2/5NH3	-10.16	57.47	-	endergonic
Cr-R012	2/7Cr2N + H2 = 4/7CrH2 + 2/7NH3	-8.45	-	-	-
Cr-R013	2/9Cr2N + H2 = 4/9CrH3 + 2/9NH3	-6.74	-	-	-
Cr-R014	Cr3H + H2 = 3CrH	1.28	-	-	-
Cr-R015	2/5Cr3H + H2 = 6/5CrH2	3.21	-	-	-
Cr-R016	1/4Cr3H + H2 = 3/4CrH3	5.14	-	-	-
Cr-R017	2Cr3N2 + H2 = 2Cr3H + 2N2	-14.68	-	-	-
Cr-R018	2/3Cr3N2 + H2 = 2CrH + 2/3N2	-13.58	228.51	-	endergonic
Cr-R019	1/3Cr3N2 + H2 = CrH2 + 1/3N2	-11.94	-	-	-
Cr-R020	2/9Cr3N2 + H2 = 2/3CrH3 + 2/9N2	-10.29	-	-	-
Cr-R021	1/3Cr3N2 + H2 = Cr + 2/3NH3	-15.22	51.64	-	endergonic
Cr-R022	2/7Cr3N2 + H2 = 2/7Cr3H + 4/7NH3	-14.68	-	-	-
Cr-R023	2/9Cr3N2 + H2 = 2/3CrH + 4/9NH3	-13.58	55.77	-	endergonic
Cr-R024	1/6Cr3N2 + H2 = 1/2CrH2 + 1/3NH3	-11.94	-	-	-
Cr-R025	2/15Cr3N2 + H2 = 2/5CrH3 + 4/15NH3	-10.29	-	-	-

Cr-R026	4/3Cr3N2 + H2 = 2Cr2N + 2/3NH3	-3.81	47.31	-	endergonic
Cr-R027	2Cr3N4 + H2 = 2Cr3H + 4N2	-25.95	-	-	-
Cr-R028	2/3Cr3N4 + H2 = 2CrH + 4/3N2	-25	228.02	-	endergonic
Cr-R029	1/3Cr3N4 + H2 = CrH2 + 2/3N2	-23.57	-	-	-
Cr-R030	2/9Cr3N4 + H2 = 2/3CrH3 + 4/9N2	-22.15	-	-	-
Cr-R031	1/6Cr3N4 + H2 = 1/2Cr + 2/3NH3	-26.43	10.4	-	endergonic
Cr-R032	2/13Cr3N4 + H2 = 2/13Cr3H + 8/13NH3	-25.95	-	-	-
Cr-R033	2/15Cr3N4 + H2 = 2/5CrH + 8/15NH3	-25	21.13	-	endergonic
Cr-R034	1/9Cr3N4 + H2 = 1/3CrH2 + 4/9NH3	-23.57	-	-	-
Cr-R035	2/21Cr3N4 + H2 = 2/7CrH3 + 8/21NH3	-22.15	-	-	-
Cr-R036	4/15Cr3N4 + H2 = 2/5Cr2N + 2/3NH3	-16.52	-15.22	-	exergonic
Cr-R037	1/3Cr3N4 + H2 = 1/3Cr3N2 + 2/3NH3	-13.21	-30.85	-	exergonic
Cr-R038	2/3Cr3N4 + H2 = 2CrN + 2/3NH3	-6.61	-100.93	-	exergonic
Cr-R039	2CrH + H2 = 2CrH2	1.9	-	-	-
Cr-R040	CrH + H2 = CrH3	3.8	-	-	-
Cr-R041	2CrH2 + H2 = 2CrH3	1.87	-	-	-
Cr-R042	6CrN + H2 = 2Cr3H + 3N2	-20.71	-	-	-
Cr-R043	2CrN + H2 = 2CrH + N2	-19.69	298.35	-	endergonic
Cr-R044	CrN + H2 = CrH2 + 1/2N2	-18.17	-	-	-
Cr-R045	2/3CrN + H2 = 2/3CrH3 + 1/3N2	-16.64	-	-	-
Cr-R046	2/3CrN + H2 = 2/3Cr + 2/3NH3	-21.22	47.51	-	endergonic
Cr-R047	3/5CrN + H2 = 1/5Cr3H + 3/5NH3	-20.71	-	-	-
Cr-R048	1/2CrN + H2 = 1/2CrH + 1/2NH3	-19.69	51.64	-	endergonic
Cr-R049	2/5CrN + H2 = 2/5CrH2 + 2/5NH3	-18.17	-	-	-
Cr-R050	1/3CrN + H2 = 1/3CrH3 + 1/3NH3	-16.64	-	-	-
Cr-R051	4/3CrN + H2 = 2/3Cr2N + 2/3NH3	-10.61	41.93	-	endergonic
Cr-R052	2CrN + H2 = 2/3Cr3N2 + 2/3NH3	-7.07	39.24	-	endergonic
Cr-R053	6CrN2 + H2 = 2Cr3H + 6N2	-34.59	-	-	-
Cr-R054	2CrN2 + H2 = 2CrH + 2N2	-33.75	181.37	259.7	exergonic
Cr-R055	CrN2 + H2 = CrH2 + N2	-32.49	-	-	-
Cr-R056	2/3CrN2 + H2 = 2/3CrH3 + 2/3N2	-31.23	-	-	-
Cr-R057	1/3CrN2 + H2 = 1/3Cr + 2/3NH3	-35.01	-11.04	-	exergonic
Cr-R058	6/19CrN2 + H2 = 2/19Cr3H + 12/19NH3	-34.59	-	-	-
Cr-R059	2/7CrN2 + H2 = 2/7CrH + 4/7NH3	-33.75	-0.32	-	endergonic
Cr-R060	1/4CrN2 + H2 = 1/4CrH2 + 1/2NH3	-32.49	-	-	-
Cr-R061	2/9CrN2 + H2 = 2/9CrH3 + 4/9NH3	-31.23	-	-	-
Cr-R062	4/9CrN2 + H2 = 2/9Cr2N + 2/3NH3	-26.26	-32.42	-	exergonic
Cr-R063	1/2CrN2 + H2 = 1/6Cr3N2 + 2/3NH3	-23.34	-42.38	-	exergonic
Cr-R064	CrN2 + H2 = 1/3Cr3N4 + 2/3NH3	-11.67	-53.92	-	exergonic
Cr-R065	2/3CrN2 + H2 = 2/3CrN + 2/3NH3	-17.51	-69.59	-	exergonic
Cr-R066	4Cr + N2 = 2Cr2N	13.47	-251.04	-	exergonic
Cr-R067	3Cr + N2 = Cr3N2	17.96	-246.71	-	exergonic
Cr-R068	3/2Cr + N2 = 1/2Cr3N4	35.92	-122.98	409.5	exergonic
Cr-R069	2Cr + N2 = 2CrN	26.94	-234.31	-	exergonic
Cr-R070	Cr + N2 = CrN2	53.88	-58.66	-	endergonic
Cr-R071	6Cr2N + N2 = 4Cr3N2	3.96	-233.71	513.8	exergonic
Cr-R072	6/5Cr2N + N2 = 4/5Cr3N4	19.78	-46.15	-	endergonic
Cr-R073	2Cr2N + N2 = 4CrN	11.87	-217.58	-	exergonic
Cr-R074	2/3Cr2N + N2 = 4/3CrN2	35.61	5.46	-	endergonic

Cr-R075	4/3Cr3H + N2 = 2Cr2N + 2/3H2	12.74	-	-	-
Cr-R076	Cr3H + N2 = Cr3N2 + 1/2H2	17.2	-	-	-
Cr-R077	1/2Cr3H + N2 = 1/2Cr3N4 + 1/4H2	35.05	-	-	-
Cr-R078	2/3Cr3H + N2 = 2CrN + 1/3H2	26.12	-	-	-
Cr-R079	1/3Cr3H + N2 = CrN2 + 1/6H2	52.89	-	-	-
Cr-R080	6Cr3H + N2 = 18Cr + 2NH3	-0.64	-	-	-
Cr-R081	12/11Cr3H + N2 = 18/11Cr2N + 4/11NH3	12.74	-	-	-
Cr-R082	6/7Cr3H + N2 = 6/7Cr3N2 + 2/7NH3	17.2	-	-	-
Cr-R083	6/13Cr3H + N2 = 6/13Cr3N4 + 2/13NH3	35.05	-	-	-
Cr-R084	3/5Cr3H + N2 = 9/5CrN + 1/5NH3	26.12	-	-	-
Cr-R085	6/19Cr3H + N2 = 18/19CrN2 + 2/19NH3	52.89	-	-	-
Cr-R086	Cr3N2 + N2 = Cr3N4	15.22	0.74	-	endergonic
Cr-R087	2Cr3N2 + N2 = 6CrN	7.61	-209.51	-	exergonic
Cr-R088	1/2Cr3N2 + N2 = 3/2CrN2	30.45	35.36	-	endergonic
Cr-R089	Cr3N4 + N2 = 3CrN2	13.21	69.97	-	endergonic
Cr-R090	4CrH + N2 = 2Cr2N + 2H2	11.31	-379.12	-	exergonic
Cr-R091	3CrH + N2 = Cr3N2 + 3/2H2	15.72	-342.77	-	exergonic
Cr-R092	3/2CrH + N2 = 1/2Cr3N4 + 3/4H2	33.33	-171.01	-	exergonic
Cr-R093	2CrH + N2 = 2CrN + H2	24.52	-298.35	-	exergonic
Cr-R094	CrH + N2 = CrN2 + 1/2H2	50.95	-90.68	259.7	exergonic
Cr-R095	6CrH + N2 = 6Cr + 2NH3	-1.9	-283.91	-	exergonic
Cr-R096	9CrH + N2 = 3Cr3H + 2NH3	-1.27	-	-	-
Cr-R097	12/5CrH + N2 = 6/5Cr2N + 4/5NH3	11.31	-264.19	-	exergonic
Cr-R098	2CrH + N2 = 2/3Cr3N2 + 2/3NH3	15.72	-259.11	-	exergonic
Cr-R099	6/5CrH + N2 = 2/5Cr3N4 + 2/5NH3	33.33	-155.17	-	exergonic
Cr-R100	3/2CrH + N2 = 3/2CrN + 1/2NH3	24.52	-246.71	-	exergonic
Cr-R101	6/7CrH + N2 = 6/7CrN2 + 2/7NH3	50.95	-90.84	247.6	exergonic
Cr-R102	4CrH2 + N2 = 2Cr2N + 4H2	9.23	-	-	-
Cr-R103	3CrH2 + N2 = Cr3N2 + 3H2	13.56	-	-	-
Cr-R104	3/2CrH2 + N2 = 1/2Cr3N4 + 3/2H2	30.84	-	-	-
Cr-R105	2CrH2 + N2 = 2CrN + 2H2	22.2	-	-	-
Cr-R106	CrH2 + N2 = CrN2 + H2	48.13	-	-	-
Cr-R107	3CrH2 + N2 = 3Cr + 2NH3	-3.73	-	-	-
Cr-R108	18/5CrH2 + N2 = 6/5Cr3H + 2NH3	-3.11	-	-	-
Cr-R109	6CrH2 + N2 = 6CrH + 2NH3	-1.87	-	-	-
Cr-R110	12/7CrH2 + N2 = 6/7Cr2N + 8/7NH3	9.23	-	-	-
Cr-R111	3/2CrH2 + N2 = 1/2Cr3N2 + NH3	13.56	-	-	-
Cr-R112	CrH2 + N2 = 1/3Cr3N4 + 2/3NH3	30.84	-	-	-
Cr-R113	6/5CrH2 + N2 = 6/5CrN + 4/5NH3	22.2	-	-	-
Cr-R114	3/4CrH2 + N2 = 3/4CrN2 + 1/2NH3	48.13	-	-	-
Cr-R115	4CrH3 + N2 = 2Cr2N + 6H2	7.23	-	-	-
Cr-R116	3CrH3 + N2 = Cr3N2 + 9/2H2	11.48	-	-	-
Cr-R117	3/2CrH3 + N2 = 1/2Cr3N4 + 9/4H2	28.45	-	-	-
Cr-R118	2CrH3 + N2 = 2CrN + 3H2	19.96	-	-	-
Cr-R119	CrH3 + N2 = CrN2 + 3/2H2	45.42	-	-	-
Cr-R120	2CrH3 + N2 = 2Cr + 2NH3	-5.5	-	-	-
Cr-R121	9/4CrH3 + N2 = 3/4Cr3H + 2NH3	-4.89	-	-	-
Cr-R122	3CrH3 + N2 = 3CrH + 2NH3	-3.66	-	-	-
Cr-R123	6CrH3 + N2 = 6CrH2 + 2NH3	-1.83	-	-	-

Cr-R124	4/3CrH3 + N2 = 2/3Cr2N + 4/3NH3	7.23	-	-	-
Cr-R125	6/5CrH3 + N2 = 2/5Cr3N2 + 6/5NH3	11.48	-	-	-
Cr-R126	6/7CrH3 + N2 = 2/7Cr3N4 + 6/7NH3	28.45	-	-	-
Cr-R127	CrH3 + N2 = CrN + NH3	19.96	-	-	-
Cr-R128	2/3CrH3 + N2 = 2/3CrN2 + 2/3NH3	45.42	-	-	-
Cr-R129	6CrN + N2 = 2Cr3N4	7.07	211	-	endergonic
Cr-R130	2CrN + N2 = 2CrN2	21.22	116.98	-	endergonic

Table S18: The Cu-based system

ID	**Reaction**	**dm_stoich [%]**	**h298 [kJ/mol]**	**T_eq [°C]**	**Type**
Cu-R01	2Cu + H2 = 2CuH	1.59	44.46	-	endergonic
Cu-R02	1/5Cu10N3 + H2 = 2CuH + 3/10N2	-4.71	-	-	-
Cu-R03	2/9Cu10N3 + H2 = 20/9Cu + 2/3NH3	-6.2	-	-	-
Cu-R04	2/19Cu10N3 + H2 = 20/19CuH + 6/19NH3	-4.71	-	-	-
Cu-R05	Cu2N + H2 = 2CuH + 1/2N2	-8.5	-	-	-
Cu-R06	2/3Cu2N + H2 = 4/3Cu + 2/3NH3	-9.93	-	-	-
Cu-R07	2/5Cu2N + H2 = 4/5CuH + 2/5NH3	-8.5	-	-	-
Cu-R08	5/3Cu2N + H2 = 1/3Cu10N3 + 2/3NH3	-3.97	-	-	-
Cu-R09	2Cu2N + H2 = 4/3Cu3N + 2/3NH3	-3.31	-	-	-
Cu-R10	2/3Cu3N + H2 = 2CuH + 1/3N2	-5.37	-4.97	-	endergonic
Cu-R11	2/3Cu3N + H2 = 2Cu + 2/3NH3	-6.84	-80.03	-	exergonic
Cu-R12	1/3Cu3N + H2 = CuH + 1/3NH3	-5.37	-17.78	78.7	exergonic
Cu-R13	20/3Cu3N + H2 = 2Cu10N3 + 2/3NH3	-0.68	-	-	-
Cu-R14	2CuN + H2 = 2CuH + N2	-16.76	-262.75	-	exergonic
Cu-R15	2/3CuN + H2 = 2/3Cu + 2/3NH3	-18.06	-133	-	exergonic
Cu-R16	1/2CuN + H2 = 1/2CuH + 1/2NH3	-16.76	-88.64	-	exergonic
Cu-R17	20/21CuN + H2 = 2/21Cu10N3 + 2/3NH3	-12.64	-	-	-
Cu-R18	4/3CuN + H2 = 2/3Cu2N + 2/3NH3	-9.03	-	-	-
Cu-R19	CuN + H2 = 1/3Cu3N + 2/3NH3	-12.04	-159.49	-	exergonic
Cu-R20	2CuN3 + H2 = 2CuH + 3N2	-38.85	-182.34	-	exergonic
Cu-R21	2/9CuN3 + H2 = 2/9Cu + 2/3NH3	-39.81	-55.8	-	exergonic
Cu-R22	1/5CuN3 + H2 = 1/5CuH + 3/5NH3	-38.85	-45.77	681.5	exergonic
Cu-R23	20/81CuN3 + H2 = 2/81Cu10N3 + 2/3NH3	-35.82	-	-	-
Cu-R24	4/15CuN3 + H2 = 2/15Cu2N + 2/3NH3	-33.17	-	-	-
Cu-R25	1/4CuN3 + H2 = 1/12Cu3N + 2/3NH3	-35.38	-52.77	-	exergonic
Cu-R26	1/3CuN3 + H2 = 1/3CuN + 2/3NH3	-26.54	-17.19	114.8	exergonic
Cu-R27	2CuN6 + H2 = 2CuH + 6N2	-56.26	-413.77	-	exergonic
Cu-R28	1/9CuN6 + H2 = 1/9Cu + 2/3NH3	-56.94	-56.05	-	exergonic
Cu-R29	2/19CuN6 + H2 = 2/19CuH + 12/19NH3	-56.26	-50.76	-	exergonic
Cu-R30	20/171CuN6 + H2 = 2/171Cu10N3 + 2/3NH3	-54.1	-	-	-
Cu-R31	4/33CuN6 + H2 = 2/33Cu2N + 2/3NH3	-52.2	-	-	-
Cu-R32	2/17CuN6 + H2 = 2/51Cu3N + 2/3NH3	-53.78	-54.64	-	exergonic
Cu-R33	2/15CuN6 + H2 = 2/15CuN + 2/3NH3	-47.45	-40.67	784.7	exergonic
Cu-R34	2/9CuN6 + H2 = 2/9CuN3 + 2/3NH3	-28.47	-56.31	-	exergonic
Cu-R35	2CuN8 + H2 = 2CuH + 8N2	-63.24	-	-	-
Cu-R36	1/12CuN8 + H2 = 1/12Cu + 2/3NH3	-63.81	-	-	-
Cu-R37	2/25CuN8 + H2 = 2/25CuH + 16/25NH3	-63.24	-	-	-
Cu-R38	20/231CuN8 + H2 = 2/231Cu10N3 + 2/3NH3	-61.42	-	-	-

Cu-R39	4/45CuN8 + H2 = 2/45Cu2N + 2/3NH3	-59.82	-	-	-
Cu-R40	2/23CuN8 + H2 = 2/69Cu3N + 2/3NH3	-61.15	-	-	-
Cu-R41	2/21CuN8 + H2 = 2/21CuN + 2/3NH3	-55.84	-	-	-
Cu-R42	2/15CuN8 + H2 = 2/15CuN3 + 2/3NH3	-39.88	-	-	-
Cu-R43	1/3CuN8 + H2 = 1/3CuN6 + 2/3NH3	-15.95	-	-	-
Cu-R44	20/3Cu + N2 = 2/3Cu10N3	6.61	-	-	-
Cu-R45	4Cu + N2 = 2Cu2N	11.02	-	-	-
Cu-R46	6Cu + N2 = 2Cu3N	7.35	148.29	-	endergonic
Cu-R47	2Cu + N2 = 2CuN	22.04	307.21	-	endergonic
Cu-R48	2/3Cu + N2 = 2/3CuN3	66.13	75.6	-	endergonic
Cu-R49	1/3Cu + N2 = 1/3CuN6	132.25	76.37	-	endergonic
Cu-R50	1/4Cu + N2 = 1/4CuN8	176.34	-	-	-
Cu-R51	Cu10N3 + N2 = 5Cu2N	4.14	-	-	-
Cu-R52	6Cu10N3 + N2 = 20Cu3N	0.69	-	-	-
Cu-R53	2/7Cu10N3 + N2 = 20/7CuN	14.47	-	-	-
Cu-R54	2/27Cu10N3 + N2 = 20/27CuN3	55.82	-	-	-
Cu-R55	2/57Cu10N3 + N2 = 20/57CuN6	117.85	-	-	-
Cu-R56	2/77Cu10N3 + N2 = 20/77CuN8	159.2	-	-	-
Cu-R57	2Cu2N + N2 = 4CuN	9.93	-	-	-
Cu-R58	2/5Cu2N + N2 = 4/5CuN3	49.64	-	-	-
Cu-R59	2/11Cu2N + N2 = 4/11CuN6	109.2	-	-	-
Cu-R60	2/15Cu2N + N2 = 4/15CuN8	148.91	-	-	-
Cu-R61	4Cu3N + N2 = 6Cu2N	3.42	-	-	-
Cu-R62	Cu3N + N2 = 3CuN	13.69	386.67	-	endergonic
Cu-R63	1/4Cu3N + N2 = 3/4CuN3	54.76	66.51	-	endergonic
Cu-R64	2/17Cu3N + N2 = 6/17CuN6	116.36	72.14	-	endergonic
Cu-R65	2/23Cu3N + N2 = 6/23CuN8	157.42	-	-	-
Cu-R66	20/3CuH + N2 = 2/3Cu10N3 + 10/3H2	4.95	-	-	-
Cu-R67	4CuH + N2 = 2Cu2N + 2H2	9.29	-	-	-
Cu-R68	6CuH + N2 = 2Cu3N + 3H2	5.67	14.91	-	exergonic
Cu-R69	2CuH + N2 = 2CuN + H2	20.14	262.75	-	endergonic
Cu-R70	2/3CuH + N2 = 2/3CuN3 + 1/3H2	63.53	60.78	-	endergonic
Cu-R71	1/3CuH + N2 = 1/3CuN6 + 1/6H2	128.63	68.96	-	endergonic
Cu-R72	1/4CuH + N2 = 1/4CuN8 + 1/8H2	172.02	-	-	-
Cu-R73	6CuH + N2 = 6Cu + 2NH3	-1.56	-225.17	-	exergonic
Cu-R74	60/19CuH + N2 = 6/19Cu10N3 + 20/19NH3	4.95	-	-	-
Cu-R75	12/5CuH + N2 = 6/5Cu2N + 4/5NH3	9.29	-	-	-
Cu-R76	3CuH + N2 = Cu3N + NH3	5.67	-38.44	408.9	exergonic
Cu-R77	3/2CuH + N2 = 3/2CuN + 1/2NH3	20.14	174.12	-	endergonic
Cu-R78	3/5CuH + N2 = 3/5CuN3 + 1/5NH3	63.53	45.52	-	endergonic
Cu-R79	6/19CuH + N2 = 6/19CuN6 + 2/19NH3	128.63	60.5	-	endergonic
Cu-R80	6/25CuH + N2 = 6/25CuN8 + 2/25NH3	172.02	-	-	-
Cu-R81	CuN + N2 = CuN3	36.12	-40.21	374.1	exergonic
Cu-R82	2/5CuN + N2 = 2/5CuN6	90.31	30.2	-	endergonic
Cu-R83	2/7CuN + N2 = 2/7CuN8	126.43	-	-	-
Cu-R84	2/3CuN3 + N2 = 2/3CuN6	39.81	77.14	-	endergonic
Cu-R85	2/5CuN3 + N2 = 2/5CuN8	66.34	-	-	-
Cu-R86	CuN6 + N2 = CuN8	18.98	-	-	-

Table S19: The Fe-based system

ID	Reaction	dm_stoich [%]	h298 [kJ/mol]	T_eq [°C]	Type
Fe-R001	6Fe + H2 = 2Fe3H	0.6	-	-	-
Fe-R002	2Fe + H2 = 2FeH	1.8	-25.94	-	endergonic
Fe-R003	2/3Fe + H2 = 2/3FeH3	5.41	38.34	-	endergonic
Fe-R004	1/2Fe + H2 = 1/2FeH4	7.22	-	-	-
Fe-R005	1/2Fe12N5 + H2 = 2Fe3H + 5/4N2	-8.92	-	-	-
Fe-R006	1/6Fe12N5 + H2 = 2FeH + 5/12N2	-7.83	-	-	-
Fe-R007	1/18Fe12N5 + H2 = 2/3FeH3 + 5/36N2	-4.56	-	-	-
Fe-R008	1/24Fe12N5 + H2 = 1/2FeH4 + 5/48N2	-2.93	-	-	-
Fe-R009	2/15Fe12N5 + H2 = 8/5Fe + 2/3NH3	-9.46	-	-	-
Fe-R010	2/19Fe12N5 + H2 = 8/19Fe3H + 10/19NH3	-8.92	-	-	-
Fe-R011	2/27Fe12N5 + H2 = 8/9FeH + 10/27NH3	-7.83	-	-	-
Fe-R012	2/51Fe12N5 + H2 = 8/17FeH3 + 10/51NH3	-4.56	-	-	-
Fe-R013	2/63Fe12N5 + H2 = 8/21FeH4 + 10/63NH3	-2.93	-	-	-
Fe-R014	2/3Fe12N5 + H2 = 8/3Fe3N + 2/3NH3	-1.89	-	-	-
Fe-R015	1/3Fe12N5 + H2 = Fe4N + 2/3NH3	-3.78	-	-	-
Fe-R016	4/21Fe12N5 + H2 = 2/7Fe8N + 2/3NH3	-6.62	-	-	-
Fe-R017	4/3Fe12N5 + H2 = 2Fe8N3 + 2/3NH3	-0.95	-	-	-
Fe-R018	1/4Fe24N11 + H2 = 2Fe3H + 11/8N2	-9.77	-	-	-
Fe-R019	1/12Fe24N11 + H2 = 2FeH + 11/24N2	-8.69	-	-	-
Fe-R020	1/36Fe24N11 + H2 = 2/3FeH3 + 11/72N2	-5.45	-	-	-
Fe-R021	1/48Fe24N11 + H2 = 1/2FeH4 + 11/96N2	-3.84	-	-	-
Fe-R022	2/33Fe24N11 + H2 = 16/11Fe + 2/3NH3	-10.31	-	-	-
Fe-R023	2/41Fe24N11 + H2 = 16/41Fe3H + 22/41NH3	-9.77	-	-	-
Fe-R024	2/57Fe24N11 + H2 = 16/19FeH + 22/57NH3	-8.69	-	-	-
Fe-R025	2/105Fe24N11 + H2 = 16/35FeH3 + 22/105NH3	-5.45	-	-	-
Fe-R026	2/129Fe24N11 + H2 = 16/43FeH4 + 22/129NH3	-3.84	-	-	-
Fe-R027	2/3Fe24N11 + H2 = 4/3Fe12N5 + 2/3NH3	-0.94	-	-	-
Fe-R028	2/9Fe24N11 + H2 = 16/9Fe3N + 2/3NH3	-2.81	-	-	-
Fe-R029	2/15Fe24N11 + H2 = 4/5Fe4N + 2/3NH3	-4.69	-	-	-
Fe-R030	1/12Fe24N11 + H2 = 1/4Fe8N + 2/3NH3	-7.5	-	-	-
Fe-R031	1/3Fe24N11 + H2 = Fe8N3 + 2/3NH3	-1.87	-	-	-
Fe-R032	3Fe2N + H2 = 2Fe3H + 3/2N2	-10.61	-	-	-
Fe-R033	Fe2N + H2 = 2FeH + 1/2N2	-9.54	-22.18	61.6	exergonic
Fe-R034	1/3Fe2N + H2 = 2/3FeH3 + 1/6N2	-6.33	39.6	-	endergonic
Fe-R035	1/4Fe2N + H2 = 1/2FeH4 + 1/8N2	-4.73	-	-	-
Fe-R036	2/3Fe2N + H2 = 4/3Fe + 2/3NH3	-11.14	-28.09	468.6	exergonic
Fe-R037	6/11Fe2N + H2 = 4/11Fe3H + 6/11NH3	-10.61	-	-	-
Fe-R038	2/5Fe2N + H2 = 4/5FeH + 2/5NH3	-9.54	-27.23	136.2	exergonic
Fe-R039	2/9Fe2N + H2 = 4/9FeH3 + 2/9NH3	-6.33	16.2	-	endergonic
Fe-R040	2/11Fe2N + H2 = 4/11FeH4 + 2/11NH3	-4.73	-	-	-
Fe-R041	4Fe2N + H2 = 2/3Fe12N5 + 2/3NH3	-1.86	-	-	-
Fe-R042	8Fe2N + H2 = 2/3Fe24N11 + 2/3NH3	-0.93	-	-	-
Fe-R043	2Fe2N + H2 = 4/3Fe3N + 2/3NH3	-3.71	-104.24	459.3	exergonic
Fe-R044	4/3Fe2N + H2 = 2/3Fe4N + 2/3NH3	-5.57	-32.97	571.6	exergonic
Fe-R045	8/9Fe2N + H2 = 2/9Fe8N + 2/3NH3	-8.36	-40.56	456.5	exergonic

Fe-R046	8/3Fe2N + H2 = 2/3Fe8N3 + 2/3NH3	-2.79	-129.81	656.3	exergonic
Fe-R047	Fe3H + H2 = 3FeH	1.2	-	-	-
Fe-R048	1/4Fe3H + H2 = 3/4FeH3	4.78	-	-	-
Fe-R049	2/11Fe3H + H2 = 6/11FeH4	6.58	-	-	-
Fe-R050	2Fe3N + H2 = 2Fe3H + N2	-7.16	-	-	-
Fe-R051	2/3Fe3N + H2 = 2FeH + 1/3N2	-6.05	14.64	-	endergonic
Fe-R052	2/9Fe3N + H2 = 2/3FeH3 + 1/9N2	-2.72	51.87	-	endergonic
Fe-R053	1/6Fe3N + H2 = 1/2FeH4 + 1/12N2	-1.05	-	-	-
Fe-R054	2/3Fe3N + H2 = 2Fe + 2/3NH3	-7.72	9.99	415.8	exergonic
Fe-R055	1/2Fe3N + H2 = 1/2Fe3H + 1/2NH3	-7.16	-	-	-
Fe-R056	1/3Fe3N + H2 = FeH + 1/3NH3	-6.05	-7.98	-	endergonic
Fe-R057	1/6Fe3N + H2 = 1/2FeH3 + 1/6NH3	-2.72	31.25	-	endergonic
Fe-R058	2/15Fe3N + H2 = 2/5FeH4 + 2/15NH3	-1.05	-	-	-
Fe-R059	8/3Fe3N + H2 = 2Fe4N + 2/3NH3	-1.93	109.57	380.7	exergonic
Fe-R060	16/15Fe3N + H2 = 2/5Fe8N + 2/3NH3	-4.82	10.38	507.1	exergonic
Fe-R061	3/2Fe4N + H2 = 2Fe3H + 3/4N2	-5.33	-	-	-
Fe-R062	1/2Fe4N + H2 = 2FeH + 1/4N2	-4.2	-20.4	-	endergonic
Fe-R063	1/6Fe4N + H2 = 2/3FeH3 + 1/12N2	-0.81	40.19	-	endergonic
Fe-R064	1/8Fe4N + H2 = 1/2FeH4 + 1/16N2	0.89	-	-	-
Fe-R065	2/3Fe4N + H2 = 8/3Fe + 2/3NH3	-5.9	-23.21	365.4	exergonic
Fe-R066	6/13Fe4N + H2 = 8/13Fe3H + 6/13NH3	-5.33	-	-	-
Fe-R067	2/7Fe4N + H2 = 8/7FeH + 2/7NH3	-4.2	-24.77	36.4	exergonic
Fe-R068	2/15Fe4N + H2 = 8/15FeH3 + 2/15NH3	-0.81	26.03	-	endergonic
Fe-R069	2/19Fe4N + H2 = 8/19FeH4 + 2/19NH3	0.89	-	-	-
Fe-R070	4/3Fe4N + H2 = 2/3Fe8N + 2/3NH3	-2.95	-55.75	365.2	exergonic
Fe-R071	3/4Fe8N + H2 = 2Fe3H + 3/8N2	-2.46	-	-	-
Fe-R072	1/4Fe8N + H2 = 2FeH + 1/8N2	-1.29	-10.97	-	endergonic
Fe-R073	1/12Fe8N + H2 = 2/3FeH3 + 1/24N2	2.21	43.34	-	endergonic
Fe-R074	1/16Fe8N + H2 = 1/2FeH4 + 1/32N2	3.96	-	-	-
Fe-R075	2/3Fe8N + H2 = 16/3Fe + 2/3NH3	-3.04	9.34	363.9	exergonic
Fe-R076	6/17Fe8N + H2 = 16/17Fe3H + 6/17NH3	-2.46	-	-	-
Fe-R077	2/11Fe8N + H2 = 16/11FeH + 2/11NH3	-1.29	-16.32	-	endergonic
Fe-R078	2/27Fe8N + H2 = 16/27FeH3 + 2/27NH3	2.21	35.12	-	endergonic
Fe-R079	2/35Fe8N + H2 = 16/35FeH4 + 2/35NH3	3.96	-	-	-
Fe-R080	3/4Fe8N3 + H2 = 2Fe3H + 9/8N2	-8.05	-	-	-
Fe-R081	1/4Fe8N3 + H2 = 2FeH + 3/8N2	-6.95	15.03	-	endergonic
Fe-R082	1/12Fe8N3 + H2 = 2/3FeH3 + 1/8N2	-3.65	52	-	endergonic
Fe-R083	1/16Fe8N3 + H2 = 1/2FeH4 + 3/32N2	-2	-	-	-
Fe-R084	2/9Fe8N3 + H2 = 16/9Fe + 2/3NH3	-8.6	5.82	-	endergonic
Fe-R085	6/35Fe8N3 + H2 = 16/35Fe3H + 18/35NH3	-8.05	-	-	-
Fe-R086	2/17Fe8N3 + H2 = 16/17FeH + 6/17NH3	-6.95	-9.13	-	endergonic
Fe-R087	2/33Fe8N3 + H2 = 16/33FeH3 + 2/11NH3	-3.65	29.47	-	endergonic
Fe-R088	2/41Fe8N3 + H2 = 16/41FeH4 + 6/41NH3	-2	-	-	-
Fe-R089	2Fe8N3 + H2 = 16/3Fe3N + 2/3NH3	-0.96	-27.52	-	endergonic
Fe-R090	2/3Fe8N3 + H2 = 4/3Fe4N + 2/3NH3	-2.87	63.88	751.2	exergonic
Fe-R091	1/3Fe8N3 + H2 = 1/3Fe8N + 2/3NH3	-5.73	4.06	-	endergonic
Fe-R092	FeH + H2 = FeH3	3.55	70.49	-	endergonic
Fe-R093	2/3FeH + H2 = 2/3FeH4	5.32	-	-	-
Fe-R094	2FeH3 + H2 = 2FeH4	1.71	-	-	-

Fe-R095	6FeN + H2 = 2Fe3H + 3N2	-19.57	-	-	-
Fe-R096	2FeN + H2 = 2FeH + N2	-18.61	95.13	-	endergonic
Fe-R097	2/3FeN + H2 = 2/3FeH3 + 1/3N2	-15.72	78.7	-	endergonic
Fe-R098	1/2FeN + H2 = 1/2FeH4 + 1/4N2	-14.28	-	-	-
Fe-R099	2/3FeN + H2 = 2/3Fe + 2/3NH3	-20.05	9.76	-	endergonic
Fe-R100	3/5FeN + H2 = 1/5Fe3H + 3/5NH3	-19.57	-	-	-
Fe-R101	1/2FeN + H2 = 1/2FeH + 1/2NH3	-18.61	0.83	-	endergonic
Fe-R102	1/3FeN + H2 = 1/3FeH3 + 1/3NH3	-15.72	24.05	-	endergonic
Fe-R103	2/7FeN + H2 = 2/7FeH4 + 2/7NH3	-14.28	-	-	-
Fe-R104	8/7FeN + H2 = 2/21Fe12N5 + 2/3NH3	-11.7	-	-	-
Fe-R105	16/13FeN + H2 = 2/39Fe24N11 + 2/3NH3	-10.86	-	-	-
Fe-R106	4/3FeN + H2 = 2/3Fe2N + 2/3NH3	-10.03	47.61	-	endergonic
Fe-R107	FeN + H2 = 1/3Fe3N + 2/3NH3	-13.37	9.65	-	endergonic
Fe-R108	8/9FeN + H2 = 2/9Fe4N + 2/3NH3	-15.04	20.75	-	endergonic
Fe-R109	16/21FeN + H2 = 2/21Fe8N + 2/3NH3	-17.55	9.82	-	endergonic
Fe-R110	16/15FeN + H2 = 2/15Fe8N3 + 2/3NH3	-12.53	12.12	-	endergonic
Fe-R111	6FeN2 + H2 = 2Fe3H + 6N2	-33.01	-	-	-
Fe-R112	2FeN2 + H2 = 2FeH + 2N2	-32.2	-	-	-
Fe-R113	2/3FeN2 + H2 = 2/3FeH3 + 2/3N2	-29.8	-	-	-
Fe-R114	1/2FeN2 + H2 = 1/2FeH4 + 1/2N2	-28.6	-	-	-
Fe-R115	1/3FeN2 + H2 = 1/3Fe + 2/3NH3	-33.41	-	-	-
Fe-R116	6/19FeN2 + H2 = 2/19Fe3H + 12/19NH3	-33.01	-	-	-
Fe-R117	2/7FeN2 + H2 = 2/7FeH + 4/7NH3	-32.2	-	-	-
Fe-R118	2/9FeN2 + H2 = 2/9FeH3 + 4/9NH3	-29.8	-	-	-
Fe-R119	1/5FeN2 + H2 = 1/5FeH4 + 2/5NH3	-28.6	-	-	-
Fe-R120	8/19FeN2 + H2 = 2/57Fe12N5 + 2/3NH3	-26.45	-	-	-
Fe-R121	16/37FeN2 + H2 = 2/111Fe24N11 + 2/3NH3	-25.75	-	-	-
Fe-R122	4/9FeN2 + H2 = 2/9Fe2N + 2/3NH3	-25.05	-	-	-
Fe-R123	2/5FeN2 + H2 = 2/15Fe3N + 2/3NH3	-27.84	-	-	-
Fe-R124	8/21FeN2 + H2 = 2/21Fe4N + 2/3NH3	-29.23	-	-	-
Fe-R125	16/45FeN2 + H2 = 2/45Fe8N + 2/3NH3	-31.32	-	-	-
Fe-R126	16/39FeN2 + H2 = 2/39Fe8N3 + 2/3NH3	-27.14	-	-	-
Fe-R127	2/3FeN2 + H2 = 2/3FeN + 2/3NH3	-16.7	-	-	-
Fe-R128	24/5Fe + N2 = 2/5Fe12N5	10.45	-	-	-
Fe-R129	48/11Fe + N2 = 2/11Fe24N11	11.5	-	-	-
Fe-R130	4Fe + N2 = 2Fe2N	12.54	-7.53	-	endergonic
Fe-R131	6Fe + N2 = 2Fe3N	8.36	-121.76	218.7	exergonic
Fe-R132	8Fe + N2 = 2Fe4N	6.27	-22.18	-	endergonic
Fe-R133	16Fe + N2 = 2Fe8N	3.14	-119.82	218.2	exergonic
Fe-R134	16/3Fe + N2 = 2/3Fe8N3	9.41	-109.26	297.7	exergonic
Fe-R135	2Fe + N2 = 2FeN	25.08	-121.07	450.3	exergonic
Fe-R136	Fe + N2 = FeN2	50.16	-	-	-
Fe-R137	4Fe12N5 + N2 = 2Fe24N11	0.95	-	-	-
Fe-R138	2Fe12N5 + N2 = 12Fe2N	1.89	-	-	-
Fe-R139	2/7Fe12N5 + N2 = 24/7FeN	13.25	-	-	-
Fe-R140	2/19Fe12N5 + N2 = 24/19FeN2	35.96	-	-	-
Fe-R141	2Fe24N11 + N2 = 24Fe2N	0.94	-	-	-
Fe-R142	2/13Fe24N11 + N2 = 48/13FeN	12.19	-	-	-
Fe-R143	2/37Fe24N11 + N2 = 48/37FeN2	34.68	-	-	-

Fe-R144	2Fe2N + N2 = 4FeN	11.14	-234.62	713.9	exergonic
Fe-R145	2/3Fe2N + N2 = 4/3FeN2	33.43	-	-	-
Fe-R146	8/5Fe3H + N2 = 2/5Fe12N5 + 4/5H2	9.79	-	-	-
Fe-R147	16/11Fe3H + N2 = 2/11Fe24N11 + 8/11H2	10.83	-	-	-
Fe-R148	4/3Fe3H + N2 = 2Fe2N + 2/3H2	11.87	-	-	-
Fe-R149	2Fe3H + N2 = 2Fe3N + H2	7.71	-	-	-
Fe-R150	8/3Fe3H + N2 = 2Fe4N + 4/3H2	5.63	-	-	-
Fe-R151	16/3Fe3H + N2 = 2Fe8N + 8/3H2	2.52	-	-	-
Fe-R152	16/9Fe3H + N2 = 2/3Fe8N3 + 8/9H2	8.75	-	-	-
Fe-R153	2/3Fe3H + N2 = 2FeN + 1/3H2	24.33	-	-	-
Fe-R154	1/3Fe3H + N2 = FeN2 + 1/6H2	49.27	-	-	-
Fe-R155	6Fe3H + N2 = 18Fe + 2NH3	-0.6	-	-	-
Fe-R156	24/19Fe3H + N2 = 6/19Fe12N5 + 8/19NH3	9.79	-	-	-
Fe-R157	48/41Fe3H + N2 = 6/41Fe24N11 + 16/41NH3	10.83	-	-	-
Fe-R158	12/11Fe3H + N2 = 18/11Fe2N + 4/11NH3	11.87	-	-	-
Fe-R159	3/2Fe3H + N2 = 3/2Fe3N + 1/2NH3	7.71	-	-	-
Fe-R160	24/13Fe3H + N2 = 18/13Fe4N + 8/13NH3	5.63	-	-	-
Fe-R161	48/17Fe3H + N2 = 18/17Fe8N + 16/17NH3	2.52	-	-	-
Fe-R162	48/35Fe3H + N2 = 18/35Fe8N3 + 16/35NH3	8.75	-	-	-
Fe-R163	3/5Fe3H + N2 = 9/5FeN + 1/5NH3	24.33	-	-	-
Fe-R164	6/19Fe3H + N2 = 18/19FeN2 + 2/19NH3	49.27	-	-	-
Fe-R165	8Fe3N + N2 = 2Fe12N5	1.93	-	-	-
Fe-R166	16/3Fe3N + N2 = 2/3Fe24N11	2.89	-	-	-
Fe-R167	4Fe3N + N2 = 6Fe2N	3.86	220.92	687.5	exergonic
Fe-R168	16Fe3N + N2 = 6Fe8N3	0.96	-9.24	-	exergonic
Fe-R169	Fe3N + N2 = 3FeN	15.43	-120.73	731.6	exergonic
Fe-R170	2/5Fe3N + N2 = 6/5FeN2	38.58	-	-	-
Fe-R171	3Fe4N + N2 = Fe12N5	3.93	-	-	-
Fe-R172	12/5Fe4N + N2 = 2/5Fe24N11	4.92	-	-	-
Fe-R173	2Fe4N + N2 = 4Fe2N	5.9	7.11	-	endergonic
Fe-R174	6Fe4N + N2 = 8Fe3N	1.97	-420.51	323.2	exergonic
Fe-R175	4Fe4N + N2 = 2Fe8N3	2.95	-283.42	466.7	exergonic
Fe-R176	2/3Fe4N + N2 = 8/3FeN	17.7	-154.04	536.2	exergonic
Fe-R177	2/7Fe4N + N2 = 8/7FeN2	41.3	-	-	-
Fe-R178	6/7Fe8N + N2 = 4/7Fe12N5	7.09	-	-	-
Fe-R179	3/4Fe8N + N2 = 1/4Fe24N11	8.11	-	-	-
Fe-R180	2/3Fe8N + N2 = 8/3Fe2N	9.12	29.9	-	endergonic
Fe-R181	6/5Fe8N + N2 = 16/5Fe3N	5.07	-122.92	219.1	exergonic
Fe-R182	2Fe8N + N2 = 4Fe4N	3.04	75.47	669.5	exergonic
Fe-R183	Fe8N + N2 = Fe8N3	6.08	-103.97	366.5	exergonic
Fe-R184	2/7Fe8N + N2 = 16/7FeN	21.28	-121.25	515.3	exergonic
Fe-R185	2/15Fe8N + N2 = 16/15FeN2	45.6	-	-	-
Fe-R186	6Fe8N3 + N2 = 4Fe12N5	0.96	-	-	-
Fe-R187	3Fe8N3 + N2 = Fe24N11	1.91	-	-	-
Fe-R188	2Fe8N3 + N2 = 8Fe2N	2.87	297.64	-	endergonic
Fe-R189	2/5Fe8N3 + N2 = 16/5FeN	14.33	-128.17	580.2	exergonic
Fe-R190	2/13Fe8N3 + N2 = 16/13FeN2	37.25	-	-	-
Fe-R191	24/5FeH + N2 = 2/5Fe12N5 + 12/5H2	8.49	-	-	-
Fe-R192	48/11FeH + N2 = 2/11Fe24N11 + 24/11H2	9.52	-	-	-

Fe-R193	4FeH + N2 = 2Fe2N + 2H2	10.55	44.36	61.6	exergonic
Fe-R194	6FeH + N2 = 2Fe3N + 3H2	6.44	-43.93	-	exergonic
Fe-R195	8FeH + N2 = 2Fe4N + 4H2	4.39	81.6	-	exergonic
Fe-R196	16FeH + N2 = 2Fe8N + 8H2	1.31	87.73	-	exergonic
Fe-R197	16/3FeH + N2 = 2/3Fe8N3 + 8/3H2	7.47	-40.07	-	exergonic
Fe-R198	2FeH + N2 = 2FeN + H2	22.86	-95.13	-	exergonic
Fe-R199	FeH + N2 = FeN2 + 1/2H2	47.5	-	-	-
Fe-R200	6FeH + N2 = 6Fe + 2NH3	-1.77	-13.96	-	exergonic
Fe-R201	9FeH + N2 = 3Fe3H + 2NH3	-1.18	-	-	-
Fe-R202	8/3FeH + N2 = 2/9Fe12N5 + 8/9NH3	8.49	-	-	-
Fe-R203	48/19FeH + N2 = 2/19Fe24N11 + 16/19NH3	9.52	-	-	-
Fe-R204	12/5FeH + N2 = 6/5Fe2N + 4/5NH3	10.55	-10.1	-	exergonic
Fe-R205	3FeH + N2 = Fe3N + NH3	6.44	-67.86	732.7	exergonic
Fe-R206	24/7FeH + N2 = 6/7Fe4N + 8/7NH3	4.39	-17.48	-	exergonic
Fe-R207	48/11FeH + N2 = 6/11Fe8N + 16/11NH3	1.31	-42.83	-	exergonic
Fe-R208	48/17FeH + N2 = 6/17Fe8N3 + 16/17NH3	7.47	-64.41	-	exergonic
Fe-R209	3/2FeH + N2 = 3/2FeN + 1/2NH3	22.86	-94.3	732.1	exergonic
Fe-R210	6/7FeH + N2 = 6/7FeN2 + 2/7NH3	47.5	-	-	-
Fe-R211	24/5FeH3 + N2 = 2/5Fe12N5 + 36/5H2	4.78	-	-	-
Fe-R212	48/11FeH3 + N2 = 2/11Fe24N11 + 72/11H2	5.77	-	-	-
Fe-R213	4FeH3 + N2 = 2Fe2N + 6H2	6.76	-237.59	-	exergonic
Fe-R214	6FeH3 + N2 = 2Fe3N + 9H2	2.79	-466.84	-	exergonic
Fe-R215	8FeH3 + N2 = 2Fe4N + 12H2	0.81	-482.29	-	exergonic
Fe-R216	16FeH3 + N2 = 2Fe8N + 24H2	-2.16	-1040.04	-	exergonic
Fe-R217	16/3FeH3 + N2 = 2/3Fe8N3 + 8H2	3.79	-416	-	exergonic
Fe-R218	2FeH3 + N2 = 2FeN + 3H2	18.66	-236.1	-	exergonic
Fe-R219	FeH3 + N2 = FeN2 + 3/2H2	42.45	-	-	-
Fe-R220	2FeH3 + N2 = 2Fe + 2NH3	-5.14	-206.82	-	exergonic
Fe-R221	9/4FeH3 + N2 = 3/4Fe3H + 2NH3	-4.57	-	-	-
Fe-R222	3FeH3 + N2 = 3FeH + 2NH3	-3.42	-303.25	-	exergonic
Fe-R223	24/17FeH3 + N2 = 2/17Fe12N5 + 24/17NH3	4.78	-	-	-
Fe-R224	48/35FeH3 + N2 = 2/35Fe24N11 + 48/35NH3	5.77	-	-	-
Fe-R225	4/3FeH3 + N2 = 2/3Fe2N + 4/3NH3	6.76	-140.39	-	exergonic
Fe-R226	3/2FeH3 + N2 = 1/2Fe3N + 3/2NH3	2.79	-185.55	-	exergonic
Fe-R227	8/5FeH3 + N2 = 2/5Fe4N + 8/5NH3	0.81	-169.89	-	exergonic
Fe-R228	16/9FeH3 + N2 = 2/9Fe8N + 16/9NH3	-2.16	-197.15	-	exergonic
Fe-R229	16/11FeH3 + N2 = 2/11Fe8N3 + 16/11NH3	3.79	-180.21	-	exergonic
Fe-R230	FeH3 + N2 = FeN + NH3	18.66	-163.95	-	exergonic
Fe-R231	2/3FeH3 + N2 = 2/3FeN2 + 2/3NH3	42.45	-	-	-
Fe-R232	24/5FeH4 + N2 = 2/5Fe12N5 + 48/5H2	3.01	-	-	-
Fe-R233	48/11FeH4 + N2 = 2/11Fe24N11 + 96/11H2	3.99	-	-	-
Fe-R234	4FeH4 + N2 = 2Fe2N + 8H2	4.96	-	-	-
Fe-R235	6FeH4 + N2 = 2Fe3N + 12H2	1.06	-	-	-
Fe-R236	8FeH4 + N2 = 2Fe4N + 16H2	-0.89	-	-	-
Fe-R237	16FeH4 + N2 = 2Fe8N + 32H2	-3.81	-	-	-
Fe-R238	16/3FeH4 + N2 = 2/3Fe8N3 + 32/3H2	2.04	-	-	-
Fe-R239	2FeH4 + N2 = 2FeN + 4H2	16.66	-	-	-
Fe-R240	FeH4 + N2 = FeN2 + 2H2	40.05	-	-	-
Fe-R241	3/2FeH4 + N2 = 3/2Fe + 2NH3	-6.73	-	-	-

Fe-R242	18/11FeH4 + N2 = 6/11Fe3H + 2NH3	-6.17	-	-	-
Fe-R243	2FeH4 + N2 = 2FeH + 2NH3	-5.05	-	-	-
Fe-R244	6FeH4 + N2 = 6FeH3 + 2NH3	-1.68	-	-	-
Fe-R245	8/7FeH4 + N2 = 2/21Fe12N5 + 32/21NH3	3.01	-	-	-
Fe-R246	48/43FeH4 + N2 = 2/43Fe24N11 + 64/43NH3	3.99	-	-	-
Fe-R247	12/11FeH4 + N2 = 6/11Fe2N + 16/11NH3	4.96	-	-	-
Fe-R248	6/5FeH4 + N2 = 2/5Fe3N + 8/5NH3	1.06	-	-	-
Fe-R249	24/19FeH4 + N2 = 6/19Fe4N + 32/19NH3	-0.89	-	-	-
Fe-R250	48/35FeH4 + N2 = 6/35Fe8N + 64/35NH3	-3.81	-	-	-
Fe-R251	48/41FeH4 + N2 = 6/41Fe8N3 + 64/41NH3	2.04	-	-	-
Fe-R252	6/7FeH4 + N2 = 6/7FeN + 8/7NH3	16.66	-	-	-
Fe-R253	3/5FeH4 + N2 = 3/5FeN2 + 4/5NH3	40.05	-	-	-
Fe-R254	2FeN + N2 = 2FeN2	20.05	-	-	-

Table S20: The Li-based system

ID	**Reaction**	**dm_stoich [%]**	**h298 [kJ/mol]**	**T_eq [°C]**	**Type**
Li-R001	2Li + H2 = 2LiH	14.52	-181.08	-	exergonic
Li-R002	2Li(H3N)4 + H2 = 2LiH + 8NH3	-89.41	-	-	-
Li-R003	1/3Li15H9N8 + H2 = 5LiH + 4/3N2	-47.07	-	-	-
Li-R004	2/15Li15H9N8 + H2 = 2Li + 16/15NH3	-53.78	-	-	-
Li-R005	1/15Li15H9N8 + H2 = LiH + 8/15NH3	-47.07	-	-	-
Li-R006	4/15Li15H9N8 + H2 = Li4HN + 17/15NH3	-28.78	-	-	-
Li-R007	2Li2HN + H2 = 4LiH + N2	-44.99	-	-	-
Li-R008	Li2HN + H2 = 2Li + NH3	-51.96	-	-	-
Li-R009	1/2Li2HN + H2 = LiH + 1/2NH3	-44.99	-	-	-
Li-R010	2Li2HN + H2 = Li4HN + NH3	-25.98	-	-	-
Li-R011	Li2N + H2 = 2LiH + 1/2N2	-43	-	-	-
Li-R012	2Li2N + H2 = 2Li2HN	3.61	-	-	-
Li-R013	4Li2N + H2 = 2Li4HN + N2	-23.31	-	-	-
Li-R014	2/3Li2N + H2 = 4/3Li + 2/3NH3	-50.23	-	-	-
Li-R015	2/5Li2N + H2 = 4/5LiH + 2/5NH3	-43	-	-	-
Li-R016	Li2N + H2 = 1/2Li4HN + 1/2NH3	-23.31	-	-	-
Li-R017	2Li2N + H2 = 4/3Li3N + 2/3NH3	-16.74	-	-	-
Li-R018	2Li3(HN)2 + H2 = 6LiH + 2N2	-53.11	-	-	-
Li-R019	2Li3(HN)2 + H2 = 2Li3H3N2	1.98	-	-	-
Li-R020	14Li3(HN)2 + H2 = 6Li7H5N4 + 2N2	-7.59	-	-	-
Li-R021	1/2Li3(HN)2 + H2 = 3/2Li + NH3	-59.06	-	-	-
Li-R022	2/7Li3(HN)2 + H2 = 6/7LiH + 4/7NH3	-53.11	-	-	-
Li-R023	2Li3(HN)2 + H2 = 2/5Li15H9N8 + 4/5NH3	-11.41	-	-	-
Li-	2Li3(HN)2 + H2 = 3Li2HN + NH3	-14.76	-	-	-

R024					
Li-R025	4/5Li3(HN)2 + H2 = 3/5Li4HN + NH3	-36.91	-	-	-
Li-R026	2Li3(HN)2 + H2 = 6/7Li7H5N4 + 4/7NH3	-7.59	-	-	-
Li-R027	2Li3(HN)2 + H2 = 2Li3N + 2NH3	-31.51	-	-	-
Li-R028	2/3Li3H3N2 + H2 = 2Li + 4/3NH3	-59.85	-	-	-
Li-R029	1/3Li3H3N2 + H2 = LiH + 2/3NH3	-54.02	-	-	-
Li-R030	4/3Li3H3N2 + H2 = Li4HN + 5/3NH3	-38.14	-	-	-
Li-R031	2/3Li3N + H2 = 2LiH + 1/3N2	-31.54	-71.38	-	exergonic
Li-R032	8/3Li3N + H2 = 2Li4HN + 1/3N2	-7.88	-	-	-
Li-R033	2/3Li3N + H2 = 2Li + 2/3NH3	-40.22	79.11	-	endergonic
Li-R034	1/3Li3N + H2 = LiH + 1/3NH3	-31.54	-50.99	454.2	exergonic
Li-R035	4/3Li3N + H2 = Li4HN + 1/3NH3	-7.88	-	-	-
Li-R036	2/3Li3N2 + H2 = 2LiH + 2/3N2	-51.17	-	-	-
Li-R037	10/9Li3N2 + H2 = 2/9Li15H9N8 + 2/9N2	-7.76	-	-	-
Li-R038	4/3Li3N2 + H2 = 2Li2HN + 1/3N2	-11.25	-	-	-
Li-R039	Li3N2 + H2 = Li3(HN)2	4.13	-	-	-
Li-R040	2/3Li3N2 + H2 = 2/3Li3H3N2	6.19	-	-	-
Li-R041	8/3Li3N2 + H2 = 2Li4HN + 5/3N2	-34.31	-	-	-
Li-R042	14/15Li3N2 + H2 = 2/5Li7H5N4 + 2/15N2	-3.77	-	-	-
Li-R043	1/3Li3N2 + H2 = Li + 2/3NH3	-57.37	-	-	-
Li-R044	2/9Li3N2 + H2 = 2/3LiH + 4/9NH3	-51.17	-	-	-
Li-R045	2/3Li3N2 + H2 = 2/15Li15H9N8 + 4/15NH3	-7.76	-	-	-
Li-R046	2/3Li3N2 + H2 = Li2HN + 1/3NH3	-11.25	-	-	-
Li-R047	4/9Li3N2 + H2 = 1/3Li4HN + 5/9NH3	-34.31	-	-	-
Li-R048	2/3Li3N2 + H2 = 2/7Li7H5N4 + 4/21NH3	-3.77	-	-	-
Li-R049	4/3Li3N2 + H2 = 2Li2N + 2/3NH3	-14.34	-	-	-
Li-R050	2/3Li3N2 + H2 = 2/3Li3N + 2/3NH3	-28.68	-	-	-
Li-R051	2/3Li4HN + H2 = 8/3LiH + 1/3N2	-25.68	-	-	-
Li-R052	Li4HN + H2 = 4Li + NH3	-35.1	-	-	-
Li-R053	1/3Li4HN + H2 = 4/3LiH + 1/3NH3	-25.68	-	-	-
Li-R054	Li7H5N4 + H2 = 7LiH + 2N2	-49.26	-	-	-
Li-R055	2/7Li7H5N4 + H2 = 2Li + 8/7NH3	-55.69	-	-	-
Li-R056	1/7Li7H5N4 + H2 = LiH + 4/7NH3	-49.26	-	-	-
Li-R057	4/7Li7H5N4 + H2 = Li4HN + 9/7NH3	-31.73	-	-	-
Li-R058	2LiH2N + H2 = 2Li + 2NH3	-69.78	364.01	-	endergonic
Li-R059	LiH2N + H2 = LiH + NH3	-65.39	91.47	-	endergonic

Li-R060	4LiH2N + H2 = Li4HN + 3NH3	-53.43	-	-	-
Li-R061	2LiN + H2 = 2LiH + N2	-62.06	-	-	-
Li-R062	10/3LiN + H2 = 2/9Li15H9N8 + 7/9N2	-28.32	-	-	-
Li-R063	4LiN + H2 = 2Li2HN + N2	-31.03	-	-	-
Li-R064	3LiN + H2 = Li3(HN)2 + 1/2N2	-19.08	-	-	-
Li-R065	2LiN + H2 = 2/3Li3H3N2 + 1/3N2	-17.48	-	-	-
Li-R066	8LiN + H2 = 2Li4HN + 3N2	-48.95	-	-	-
Li-R067	14/5LiN + H2 = 2/5Li7H5N4 + 3/5N2	-25.22	-	-	-
Li-R068	LiN + H2 = LiH2N	9.62	-	-	-
Li-R069	2/3LiN + H2 = 2/3Li + 2/3NH3	-66.87	-	-	-
Li-R070	1/2LiN + H2 = 1/2LiH + 1/2NH3	-62.06	-	-	-
Li-R071	LiN + H2 = 1/15Li15H9N8 + 7/15NH3	-28.32	-	-	-
Li-R072	LiN + H2 = 1/2Li2HN + 1/2NH3	-31.03	-	-	-
Li-R073	6/5LiN + H2 = 2/5Li3(HN)2 + 2/5NH3	-19.08	-	-	-
Li-R074	LiN + H2 = 1/3Li3H3N2 + 1/3NH3	-17.48	-	-	-
Li-R075	4/5LiN + H2 = 1/5Li4HN + 3/5NH3	-48.95	-	-	-
Li-R076	LiN + H2 = 1/7Li7H5N4 + 3/7NH3	-25.22	-	-	-
Li-R077	4/3LiN + H2 = 2/3Li2N + 2/3NH3	-33.43	-	-	-
Li-R078	LiN + H2 = 1/3Li3N + 2/3NH3	-44.58	-	-	-
Li-R079	2LiN + H2 = 2/3Li3N2 + 2/3NH3	-22.29	-	-	-
Li-R080	2LiN3 + H2 = 2LiH + 3N2	-83.77	-22.23	-	exergonic
Li-R081	10/3LiN3 + H2 = 2/9Li15H9N8 + 37/9N2	-69.33	-	-	-
Li-R082	4LiN3 + H2 = 2Li2HN + 5N2	-70.49	-	-	-
Li-R083	3LiN3 + H2 = Li3(HN)2 + 7/2N2	-65.38	-	-	-
Li-R084	2LiN3 + H2 = 2/3Li3H3N2 + 7/3N2	-64.69	-	-	-
Li-R085	8LiN3 + H2 = 2Li4HN + 11N2	-78.16	-	-	-
Li-R086	14/5LiN3 + H2 = 2/5Li7H5N4 + 17/5N2	-68.01	-	-	-
Li-R087	LiN3 + H2 = LiH2N + N2	-53.1	-148.48	-	exergonic
Li-R088	2/9LiN3 + H2 = 2/9Li + 2/3NH3	-85.83	-12.95	371	exergonic
Li-R089	1/5LiN3 + H2 = 1/5LiH + 3/5NH3	-83.77	-29.76	557.2	exergonic
Li-R090	1/4LiN3 + H2 = 1/60Li15H9N8 + 37/60NH3	-69.33	-	-	-
Li-R091	1/4LiN3 + H2 = 1/8Li2HN + 5/8NH3	-70.49	-	-	-
Li-R092	6/23LiN3 + H2 = 2/23Li3(HN)2 + 14/23NH3	-65.38	-	-	-
Li-R093	1/4LiN3 + H2 = 1/12Li3H3N2 + 7/12NH3	-64.69	-	-	-
Li-R094	4/17LiN3 + H2 = 1/17Li4HN + 11/17NH3	-78.16	-	-	-
Li-R095	1/4LiN3 + H2 = 1/28Li7H5N4 + 17/28NH3	-68.01	-	-	-

Li-R096	1/4LiN3 + H2 = 1/4LiH2N + 1/2NH3	-53.1	-60.07	-	exergonic
Li-R097	4/15LiN3 + H2 = 2/15Li2N + 2/3NH3	-71.52	-	-	-
Li-R098	1/4LiN3 + H2 = 1/12Li3N + 2/3NH3	-76.29	-24.45	608.4	exergonic
Li-R099	2/7LiN3 + H2 = 2/21Li3N2 + 2/3NH3	-66.75	-	-	-
Li-R100	1/3LiN3 + H2 = 1/3LiN + 2/3NH3	-57.22	-	-	-
Li-R101	4Li + N2 = 2Li2N	100.91	-	-	-
Li-R102	6Li + N2 = 2Li3N	67.28	-329.11	-	exergonic
Li-R103	3Li + N2 = Li3N2	134.55	-	-	-
Li-R104	2Li + N2 = 2LiN	201.83	-	-	-
Li-R105	2/3Li + N2 = 2/3LiN3	605.49	-52.95	82.9	exergonic
Li-R106	6Li(H3N)4 + N2 = 2/5Li15H9N8 + 114/5NH3	-80	-	-	-
Li-R107	6Li(H3N)4 + N2 = 3Li2HN + 23NH3	-80.75	-	-	-
Li-R108	9/2Li(H3N)4 + N2 = 3/2Li3(HN)2 + 17NH3	-77.42	-	-	-
Li-R109	6Li(H3N)4 + N2 = 2Li3H3N2 + 22NH3	-76.97	-	-	-
Li-R110	12Li(H3N)4 + N2 = 3Li4HN + 47NH3	-85.75	-	-	-
Li-R111	6Li(H3N)4 + N2 = 6/7Li7H5N4 + 158/7NH3	-79.13	-	-	-
Li-R112	6Li(H3N)4 + N2 = 6LiH2N + 20NH3	-69.41	-	-	-
Li-R113	4Li(H3N)4 + N2 = 2Li2N + 16NH3	-81.42	-	-	-
Li-R114	6Li(H3N)4 + N2 = 2Li3N + 24NH3	-84.53	-	-	-
Li-R115	3Li(H3N)4 + N2 = Li3N2 + 12NH3	-78.31	-	-	-
Li-R116	2Li(H3N)4 + N2 = 2LiN + 8NH3	-72.09	-	-	-
Li-R117	2/3Li(H3N)4 + N2 = 2/3LiN3 + 8/3NH3	-34.77	-	-	-
Li-R118	Li15H9N8 + N2 = 5Li3N2 + 9/2H2	8.41	-	-	-
Li-R119	2/7Li15H9N8 + N2 = 30/7LiN + 9/7H2	39.51	-	-	-
Li-R120	2/37Li15H9N8 + N2 = 30/37LiN3 + 9/37H2	226.08	-	-	-
Li-R121	4/5Li15H9N8 + N2 = 6Li2N + 12/5NH3	-7.14	-	-	-
Li-R122	2/5Li15H9N8 + N2 = 2Li3N2 + 6/5NH3	8.41	-	-	-
Li-R123	1/5Li15H9N8 + N2 = 3LiN + 3/5NH3	39.51	-	-	-
Li-R124	1/20Li15H9N8 + N2 = 3/4LiN3 + 3/20NH3	226.08	-	-	-
Li-R125	6Li2HN + N2 = 4Li3N2 + 3H2	12.67	-	-	-
Li-R126	2Li2HN + N2 = 4LiN + H2	44.99	-	-	-
Li-R127	2/5Li2HN + N2 = 4/5LiN3 + 1/5H2	238.89	-	-	-
Li-R128	6Li2HN + N2 = 6Li2N + 2NH3	-3.49	-	-	-
Li-R129	3Li2HN + N2 = 2Li3N2 + NH3	12.67	-	-	-
Li-R130	3/2Li2HN + N2 = 3LiN + 1/2NH3	44.99	-	-	-
Li-R131	3/8Li2HN + N2 = 3/4LiN3 + 1/8NH3	238.89	-	-	-

Li-R132	6Li2N + N2 = 4Li3N2	16.74	-	-	-
Li-R133	2Li2N + N2 = 4LiN	50.23	-	-	-
Li-R134	2/5Li2N + N2 = 4/5LiN3	251.14	-	-	-
Li-R135	2Li3(HN)2 + N2 = 6LiN + 2H2	23.58	-	-	-
Li-R136	2/7Li3(HN)2 + N2 = 6/7LiN3 + 2/7H2	188.86	-	-	-
Li-R137	12Li3(HN)2 + N2 = 18Li2N + 8NH3	-17.74	-	-	-
Li-R138	3Li3(HN)2 + N2 = 3Li3N2 + 2NH3	-3.96	-	-	-
Li-R139	6/5Li3(HN)2 + N2 = 18/5LiN + 4/5NH3	23.58	-	-	-
Li-R140	6/23Li3(HN)2 + N2 = 18/23LiN3 + 4/23NH3	188.86	-	-	-
Li-R141	2Li3H3N2 + N2 = 6LiN + 3H2	21.18	-	-	-
Li-R142	2/7Li3H3N2 + N2 = 6/7LiN3 + 3/7H2	183.24	-	-	-
Li-R143	Improbable stoichiometric coefficients	-16.42	-	-	-
Li-R144	6Li3H3N2 + N2 = 6Li3(HN)2 + 2NH3	-1.94	-	-	-
Li-R145	Improbable stoichiometric coefficients	-9.38	-	-	-
Li-R146	4Li3H3N2 + N2 = 6Li2N + 4NH3	-19.34	-	-	-
Li-R147	2Li3H3N2 + N2 = 2Li3N2 + 2NH3	-5.83	-	-	-
Li-R148	Li3H3N2 + N2 = 3LiN + NH3	21.18	-	-	-
Li-R149	1/4Li3H3N2 + N2 = 3/4LiN3 + 1/4NH3	183.24	-	-	-
Li-R150	4Li3N + N2 = 6Li2N	20.11	-	-	-
Li-R151	2Li3N + N2 = 2Li3N2	40.22	-	-	-
Li-R152	Li3N + N2 = 3LiN	80.44	-	-	-
Li-R153	1/4Li3N + N2 = 3/4LiN3	321.75	-18.43	-	endergonic
Li-R154	2Li3N2 + N2 = 6LiN	28.68	-	-	-
Li-R155	2/7Li3N2 + N2 = 6/7LiN3	200.78	-	-	-
Li-R156	2Li4HN + N2 = 4Li2N + H2	30.39	-	-	-
Li-R157	6Li4HN + N2 = 8Li3N + 3H2	8.56	-	-	-
Li-R158	6/5Li4HN + N2 = 8/5Li3N2 + 3/5H2	52.22	-	-	-
Li-R159	2/3Li4HN + N2 = 8/3LiN + 1/3H2	95.88	-	-	-
Li-R160	2/11Li4HN + N2 = 8/11LiN3 + 1/11H2	357.85	-	-	-
Li-R161	3/2Li4HN + N2 = 3Li2N + 1/2NH3	30.39	-	-	-
Li-R162	3Li4HN + N2 = 4Li3N + NH3	8.56	-	-	-
Li-R163	Li4HN + N2 = 4/3Li3N2 + 1/3NH3	52.22	-	-	-
Li-R164	3/5Li4HN + N2 = 12/5LiN + 1/5NH3	95.88	-	-	-
Li-R165	3/17Li4HN + N2 = 12/17LiN3 + 1/17NH3	357.85	-	-	-
Li-R166	3Li7H5N4 + N2 = 7Li3(HN)2 + 1/2H2	8.21	-	-	-
Li-R167	3Li7H5N4 + N2 = 7Li3N2 + 15/2H2	3.92	-	-	-

Li-R168	2/3Li7H5N4 + N2 = 14/3LiN + 5/3H2	33.73	-	-	-
Li-R169	2/17Li7H5N4 + N2 = 14/17LiN3 + 5/17H2	212.57	-	-	-
Li-R170	18/7Li7H5N4 + N2 = 6Li3(HN)2 + 2/7NH3	8.21	-	-	-
Li-R171	12/7Li7H5N4 + N2 = 6Li2N + 20/7NH3	-10.98	-	-	-
Li-R172	6/7Li7H5N4 + N2 = 2Li3N2 + 10/7NH3	3.92	-	-	-
Li-R173	3/7Li7H5N4 + N2 = 3LiN + 5/7NH3	33.73	-	-	-
Li-R174	3/28Li7H5N4 + N2 = 3/4LiN3 + 5/28NH3	212.57	-	-	-
Li-R175	15/4LiH + N2 = 1/4Li15H9N8 + 3/4H2	88.92	-	-	-
Li-R176	4LiH + N2 = 2Li2HN + H2	81.78	-	-	-
Li-R177	3LiH + N2 = Li3(HN)2 + 1/2H2	113.26	-	-	-
Li-R178	3LiH + N2 = Li3H3N2	117.49	-	-	-
Li-R179	8LiH + N2 = 2Li4HN + 3H2	34.55	-	-	-
Li-R180	7/2LiH + N2 = 1/2Li7H5N4 + 1/2H2	97.08	-	-	-
Li-R181	4LiH + N2 = 2Li2N + 2H2	75.43	-	-	-
Li-R182	6LiH + N2 = 2Li3N + 3H2	46.06	214.13	-	endergonic
Li-R183	3LiH + N2 = Li3N2 + 3/2H2	104.81	-	-	-
Li-R184	2LiH + N2 = 2LiN + H2	163.55	-	-	-
Li-R185	2/3LiH + N2 = 2/3LiN3 + 1/3H2	516.02	7.41	-	endergonic
Li-R186	6LiH + N2 = 6Li + 2NH3	-12.68	451.45	-	endergonic
Li-R187	3LiH + N2 = 1/5Li15H9N8 + 2/5NH3	88.92	-	-	-
Li-R188	3LiH + N2 = 3/2Li2HN + 1/2NH3	81.78	-	-	-
Li-R189	18/7LiH + N2 = 6/7Li3(HN)2 + 2/7NH3	113.26	-	-	-
Li-R190	4LiH + N2 = Li4HN + NH3	34.55	-	-	-
Li-R191	3LiH + N2 = 3/7Li7H5N4 + 2/7NH3	97.08	-	-	-
Li-R192	12/5LiH + N2 = 6/5Li2N + 4/5NH3	75.43	-	-	-
Li-R193	3LiH + N2 = Li3N + NH3	46.06	61.17	-	endergonic
Li-R194	2LiH + N2 = 2/3Li3N2 + 2/3NH3	104.81	-	-	-
Li-R195	3/2LiH + N2 = 3/2LiN + 1/2NH3	163.55	-	-	-
Li-R196	3/5LiH + N2 = 3/5LiN3 + 1/5NH3	516.02	-2.51	-	endergonic
Li-R197	LiH2N + N2 = LiN3 + H2	113.22	148.48	-	endergonic
Li-R198	18LiH2N + N2 = 6Li3(HN)2 + 8NH3	-26.19	-	-	-
Li-R199	12LiH2N + N2 = 6Li2N + 8NH3	-39.28	-	-	-
Li-R200	6LiH2N + N2 = 2Li3N2 + 4NH3	-29.11	-	-	-
Li-R201	3LiH2N + N2 = 3LiN + 2NH3	-8.78	-	-	-
Li-R202	3/4LiH2N + N2 = 3/4LiN3 + 1/2NH3	113.22	88.41	-	endergonic
Li-R203	LiN + N2 = LiN3	133.74	-	-	-

Table S21: The Mn-based system

ID	Reaction	dm_stoich [%]	h298 [kJ/mol]	T_eq [°C]	Type
Mn-R01	2Mn + H2 = 2MnH	1.83	-	-	-
Mn-R02	1/9Mn(H15N8)2 + H2 = 1/9Mn + 16/9NH3	-82.24	-	-	-
Mn-R03	2/19Mn(H15N8)2 + H2 = 2/19MnH + 32/19NH3	-81.91	-	-	-
Mn-R04	1/8Mn(H15N8)2 + H2 = 1/8Mn(H2N)2 + 7/4NH3	-71.88	-	-	-
Mn-R05	4/33Mn(H15N8)2 + H2 = 2/33Mn2N + 62/33NH3	-79.97	-	-	-
Mn-R06	1/8Mn(H15N8)2 + H2 = 1/24Mn3N2 + 23/12NH3	-79.22	-	-	-
Mn-R07	1/7Mn(H15N8)2 + H2 = 1/21Mn3N4 + 44/21NH3	-76.2	-	-	-
Mn-R08	8/69Mn(H15N8)2 + H2 = 2/69Mn4N + 42/23NH3	-81.11	-	-	-
Mn-R09	2/15Mn(H15N8)2 + H2 = 2/15MnN + 2NH3	-77.71	-	-	-
Mn-R10	5/42Mn(H15N8)2 + H2 = 1/42Mn5N2 + 13/7NH3	-80.43	-	-	-
Mn-R11	Mn(H2N)2 + H2 = Mn + 2NH3	-36.84	-	-	-
Mn-R12	2/3Mn(H2N)2 + H2 = 2/3MnH + 4/3NH3	-35.68	-	-	-
Mn-R13	4Mn(H2N)2 + H2 = 2Mn2N + 6NH3	-28.79	-	-	-
Mn-R14	8/5Mn(H2N)2 + H2 = 2/5Mn4N + 14/5NH3	-32.82	-	-	-
Mn-R15	5/2Mn(H2N)2 + H2 = 1/2Mn5N2 + 4NH3	-30.4	-	-	-
Mn-R16	Mn2N + H2 = 2MnH + 1/2N2	-9.68	-	-	-
Mn-R17	2/3Mn2N + H2 = 4/3Mn + 2/3NH3	-11.31	53.44	-	endergonic
Mn-R18	2/5Mn2N + H2 = 4/5MnH + 2/5NH3	-9.68	-	-	-
Mn-R19	4/3Mn2N + H2 = 2/3Mn4N + 2/3NH3	-5.65	51.69	-	endergonic
Mn-R20	10/3Mn2N + H2 = 4/3Mn5N2 + 2/3NH3	-2.26	117.28	-	endergonic
Mn-R21	2/3Mn3N2 + H2 = 2MnH + 2/3N2	-12.96	-	-	-
Mn-R22	1/3Mn3N2 + H2 = Mn + 2/3NH3	-14.53	33.28	-	endergonic
Mn-R23	2/9Mn3N2 + H2 = 2/3MnH + 4/9NH3	-12.96	-	-	-
Mn-R24	4/3Mn3N2 + H2 = 2Mn2N + 2/3NH3	-3.63	-27.18	96.8	exergonic
Mn-R25	8/15Mn3N2 + H2 = 2/5Mn4N + 2/3NH3	-9.08	20.15	-	endergonic
Mn-R26	5/6Mn3N2 + H2 = 1/2Mn5N2 + 2/3NH3	-5.81	26.99	-	endergonic
Mn-R27	2/3Mn3N4 + H2 = 2MnH + 4/3N2	-24	-	-	-
Mn-R28	1/6Mn3N4 + H2 = 1/2Mn + 2/3NH3	-25.37	-	-	-
Mn-R29	2/15Mn3N4 + H2 = 2/5MnH + 8/15NH3	-24	-	-	-
Mn-R30	4/15Mn3N4 + H2 = 2/5Mn2N + 2/3NH3	-15.86	-	-	-
Mn-R31	1/3Mn3N4 + H2 = 1/3Mn3N2 + 2/3NH3	-12.69	-	-	-
Mn-R32	8/39Mn3N4 + H2 = 2/13Mn4N + 2/3NH3	-20.61	-	-	-
Mn-R33	2/3Mn3N4 + H2 = 2MnN + 2/3NH3	-6.34	-	-	-

Mn-R34	5/21Mn3N4 + H2 = 1/7Mn5N2 + 2/3NH3	-17.76	-	-	-
Mn-R35	1/2Mn4N + H2 = 2MnH + 1/4N2	-4.27	-	-	-
Mn-R36	2/3Mn4N + H2 = 8/3Mn + 2/3NH3	-5.99	55.18	-	endergonic
Mn-R37	2/7Mn4N + H2 = 8/7MnH + 2/7NH3	-4.27	-	-	-
Mn-R38	2/5Mn5N2 + H2 = 2MnH + 2/5N2	-7.59	-	-	-
Mn-R39	1/3Mn5N2 + H2 = 5/3Mn + 2/3NH3	-9.25	37.48	-	endergonic
Mn-R40	2/11Mn5N2 + H2 = 10/11MnH + 4/11NH3	-7.59	-	-	-
Mn-R41	8/9Mn5N2 + H2 = 10/9Mn4N + 2/3NH3	-3.47	7.97	-	endergonic
Mn-R42	2MnN + H2 = 2MnH + N2	-18.85	-	-	-
Mn-R43	2/3MnN + H2 = 2/3Mn + 2/3NH3	-20.32	9.48	-	endergonic
Mn-R44	1/2MnN + H2 = 1/2MnH + 1/2NH3	-18.85	-	-	-
Mn-R45	4/3MnN + H2 = 2/3Mn2N + 2/3NH3	-10.16	-34.48	624	exergonic
Mn-R46	2MnN + H2 = 2/3Mn3N2 + 2/3NH3	-6.77	-38.13	-	exergonic
Mn-R47	8/9MnN + H2 = 2/9Mn4N + 2/3NH3	-15.24	-5.76	125.4	exergonic
Mn-R48	10/9MnN + H2 = 2/9Mn5N2 + 2/3NH3	-12.19	-9.19	272.6	exergonic
Mn-R49	4Mn + N2 = 2Mn2N	12.75	-252.1	-	exergonic
Mn-R50	3Mn + N2 = Mn3N2	17	-191.64	-	exergonic
Mn-R51	3/2Mn + N2 = 1/2Mn3N4	33.99	-	-	-
Mn-R52	8Mn + N2 = 2Mn4N	6.37	-257.33	-	exergonic
Mn-R53	2Mn + N2 = 2MnN	25.5	-120.23	496.6	exergonic
Mn-R54	5Mn + N2 = Mn5N2	10.2	-204.22	-	exergonic
Mn-R55	3Mn(H2N)2 + N2 = Mn3N4 + 4NH3	-15.37	-	-	-
Mn-R56	6Mn(H2N)2 + N2 = 6MnN + 8NH3	-20.74	-	-	-
Mn-R57	6Mn2N + N2 = 4Mn3N2	3.77	-10.26	-	exergonic
Mn-R58	6/5Mn2N + N2 = 4/5Mn3N4	18.84	-	-	-
Mn-R59	2Mn2N + N2 = 4MnN	11.31	11.65	-	endergonic
Mn-R60	Mn3N2 + N2 = Mn3N4	14.53	-	-	-
Mn-R61	2Mn3N2 + N2 = 6MnN	7.26	22.6	-	endergonic
Mn-R62	2Mn4N + N2 = 4Mn2N	5.99	-246.87	639.4	exergonic
Mn-R63	6/5Mn4N + N2 = 8/5Mn3N2	9.99	-152.23	-	exergonic
Mn-R64	6/13Mn4N + N2 = 8/13Mn3N4	25.97	-	-	-
Mn-R65	2/3Mn4N + N2 = 8/3MnN	17.98	-74.52	204	exergonic
Mn-R66	10/3Mn4N + N2 = 8/3Mn5N2	3.6	-115.7	450.4	exergonic
Mn-R67	4Mn5N2 + N2 = 10Mn2N	2.31	-443.62	690.4	exergonic
Mn-R68	3/2Mn5N2 + N2 = 5/2Mn3N2	6.17	-172.77	-	exergonic
Mn-R69	3/7Mn5N2 + N2 = 5/7Mn3N4	21.59	-	-	-

Mn-R70	2/3Mn5N2 + N2 = 10/3MnN	13.88	-64.23	144.9	exergonic
Mn-R71	4MnH + N2 = 2Mn2N + 2H2	10.72	-	-	-
Mn-R72	3MnH + N2 = Mn3N2 + 3/2H2	14.89	-	-	-
Mn-R73	3/2MnH + N2 = 1/2Mn3N4 + 3/4H2	31.58	-	-	-
Mn-R74	8MnH + N2 = 2Mn4N + 4H2	4.46	-	-	-
Mn-R75	2MnH + N2 = 2MnN + H2	23.23	-	-	-
Mn-R76	5MnH + N2 = Mn5N2 + 5/2H2	8.21	-	-	-
Mn-R77	6MnH + N2 = 6Mn + 2NH3	-1.8	-	-	-
Mn-R78	12/5MnH + N2 = 6/5Mn2N + 4/5NH3	10.72	-	-	-
Mn-R79	2MnH + N2 = 2/3Mn3N2 + 2/3NH3	14.89	-	-	-
Mn-R80	6/5MnH + N2 = 2/5Mn3N4 + 2/5NH3	31.58	-	-	-
Mn-R81	24/7MnH + N2 = 6/7Mn4N + 8/7NH3	4.46	-	-	-
Mn-R82	3/2MnH + N2 = 3/2MnN + 1/2NH3	23.23	-	-	-
Mn-R83	30/11MnH + N2 = 6/11Mn5N2 + 10/11NH3	8.21	-	-	-
Mn-R84	6MnN + N2 = 2Mn3N4	6.77	-	-	-

Table S22: The Mo-based system

ID	**Reaction**	**dm_stoich [%]**	**h298 [kJ/mol]**	**T_eq [°C]**	**Type**
Mo-R001	6Mo + H2 = 2Mo3H	0.35	656.27	-	endergonic
Mo-R002	2Mo + H2 = 2MoH	1.05	152.06	-	endergonic
Mo-R003	2/5Mo15N16 + H2 = 2Mo3H + 16/5N2	-13.17	-	-	-
Mo-R004	2/15Mo15N16 + H2 = 2MoH + 16/15N2	-12.56	-	-	-
Mo-R005	1/24Mo15N16 + H2 = 5/8Mo + 2/3NH3	-13.47	-	-	-
Mo-R006	2/53Mo15N16 + H2 = 10/53Mo3H + 32/53NH3	-13.17	-	-	-
Mo-R007	2/63Mo15N16 + H2 = 10/21MoH + 32/63NH3	-12.56	-	-	-
Mo-R008	4/51Mo15N16 + H2 = 10/17Mo2N + 2/3NH3	-7.16	-	-	-
Mo-R009	1/9Mo15N16 + H2 = 5/9Mo3N2 + 2/3NH3	-5.05	-	-	-
Mo-R010	2/3Mo15N16 + H2 = 10MoN + 2/3NH3	-0.84	-	-	-
Mo-R011	1/24Mo15N16 + H2 = 5/16Mo2 + 2/3NH3	-13.47	-	-	-
Mo-R012	3Mo2 + H2 = 2Mo3H	0.35	-446.23	389.5	exergonic
Mo-R013	Mo2 + H2 = 2MoH	1.05	-215.44	416.4	exergonic
Mo-R014	3Mo2N + H2 = 2Mo3H + 3/2N2	-6.48	901.03	-	endergonic
Mo-R015	Mo2N + H2 = 2MoH + 1/2N2	-5.82	233.64	-	endergonic
Mo-R016	2/3Mo2N + H2 = 4/3Mo + 2/3NH3	-6.8	23.79	-	endergonic
Mo-R017	6/11Mo2N + H2 = 4/11Mo3H + 6/11NH3	-6.48	138.79	-	endergonic
Mo-R018	2/5Mo2N + H2 = 4/5MoH + 2/5NH3	-5.82	75.1	-	endergonic
Mo-R019	2/3Mo2N + H2 = 2/3Mo2 + 2/3NH3	-6.8	268.79	-	endergonic
Mo-R020	3Mo2N3 + H2 = 2Mo3H + 9/2N2	-17.68	-	-	-
Mo-R021	Mo2N3 + H2 = 2MoH + 3/2N2	-17.1	-	-	-
Mo-R022	2/9Mo2N3 + H2 = 4/9Mo + 2/3NH3	-17.96	-	-	-
Mo-R023	6/29Mo2N3 + H2 = 4/29Mo3H + 18/29NH3	-17.68	-	-	-
Mo-R024	2/11Mo2N3 + H2 = 4/11MoH + 6/11NH3	-17.1	-	-	-
Mo-R025	10/13Mo2N3 + H2 = 4/39Mo15N16 + 2/3NH3	-5.19	-	-	-

Mo-R026	1/3Mo2N3 + H2 = 1/3Mo2N + 2/3NH3	-11.98	-	-	-
Mo-R027	2/5Mo2N3 + H2 = 4/15Mo3N2 + 2/3NH3	-9.98	-	-	-
Mo-R028	2/3Mo2N3 + H2 = 4/3MoN + 2/3NH3	-5.99	-	-	-
Mo-R029	2/9Mo2N3 + H2 = 2/9Mo2 + 2/3NH3	-17.96	-	-	-
Mo-R030	Mo3H + H2 = 3MoH	0.7	-100.05	485.6	exergonic
Mo-R031	2Mo3N2 + H2 = 2Mo3H + 2N2	-8.55	-	-	-
Mo-R032	2/3Mo3N2 + H2 = 2MoH + 2/3N2	-7.91	-	-	-
Mo-R033	1/3Mo3N2 + H2 = Mo + 2/3NH3	-8.87	-	-	-
Mo-R034	2/7Mo3N2 + H2 = 2/7Mo3H + 4/7NH3	-8.55	-	-	-
Mo-R035	2/9Mo3N2 + H2 = 2/3MoH + 4/9NH3	-7.91	-	-	-
Mo-R036	4/3Mo3N2 + H2 = 2Mo2N + 2/3NH3	-2.22	-	-	-
Mo-R037	1/3Mo3N2 + H2 = 1/2Mo2 + 2/3NH3	-8.87	-	-	-
Mo-R038	6MoN + H2 = 2Mo3H + 3N2	-12.43	901.02	-	endergonic
Mo-R039	2MoN + H2 = 2MoH + N2	-11.82	233.64	-	endergonic
Mo-R040	2/3MoN + H2 = 2/3Mo + 2/3NH3	-12.74	-3.4	293	exergonic
Mo-R041	3/5MoN + H2 = 1/5Mo3H + 3/5NH3	-12.43	62.56	-	endergonic
Mo-R042	1/2MoN + H2 = 1/2MoH + 1/2NH3	-11.82	35.46	-	endergonic
Mo-R043	4/3MoN + H2 = 2/3Mo2N + 2/3NH3	-6.37	-30.6	-	exergonic
Mo-R044	2MoN + H2 = 2/3Mo3N2 + 2/3NH3	-4.25	-	-	-
Mo-R045	2/3MoN + H2 = 1/3Mo2 + 2/3NH3	-12.74	119.1	-	endergonic
Mo-R046	6MoN2 + H2 = 2Mo3H + 6N2	-22.33	822.74	-	endergonic
Mo-R047	2MoN2 + H2 = 2MoH + 2N2	-21.79	207.55	-	endergonic
Mo-R048	1/3MoN2 + H2 = 1/3Mo + 2/3NH3	-22.6	-21.35	520.4	exergonic
Mo-R049	6/19MoN2 + H2 = 2/19Mo3H + 12/19NH3	-22.33	14.31	-	endergonic
Mo-R050	2/7MoN2 + H2 = 2/7MoH + 4/7NH3	-21.79	3.42	-	endergonic
Mo-R051	5/7MoN2 + H2 = 1/21Mo15N16 + 2/3NH3	-10.55	-	-	-
Mo-R052	4/9MoN2 + H2 = 2/9Mo2N + 2/3NH3	-16.95	-36.4	788.7	exergonic
Mo-R053	4/3MoN2 + H2 = 2/3Mo2N3 + 2/3NH3	-5.65	-	-	-
Mo-R054	1/2MoN2 + H2 = 1/6Mo3N2 + 2/3NH3	-15.07	-	-	-
Mo-R055	2/3MoN2 + H2 = 2/3MoN + 2/3NH3	-11.3	-39.3	568	exergonic
Mo-R056	1/3MoN2 + H2 = 1/6Mo2 + 2/3NH3	-22.6	39.9	-	endergonic
Mo-R057	15/8Mo + N2 = 1/8Mo15N16	15.57	-	-	-
Mo-R058	4Mo + N2 = 2Mo2N	7.3	-163.18	686.8	exergonic
Mo-R059	4/3Mo + N2 = 2/3Mo2N3	21.9	-	-	-
Mo-R060	3Mo + N2 = Mo3N2	9.73	-	-	-
Mo-R061	2Mo + N2 = 2MoN	14.6	-81.59	165.1	exergonic
Mo-R062	Mo + N2 = MoN2	29.2	-27.75	-	endergonic
Mo-R063	4/13Mo15N16 + N2 = 30/13Mo2N3	5.47	-	-	-
Mo-R064	1/7Mo15N16 + N2 = 15/7MoN2	11.79	-	-	-
Mo-R065	15/16Mo2 + N2 = 1/8Mo15N16	15.57	-	-	-
Mo-R066	2Mo2 + N2 = 2Mo2N	7.3	-898.18	-	exergonic
Mo-R067	2/3Mo2 + N2 = 2/3Mo2N3	21.9	-	-	-
Mo-R068	3/2Mo2 + N2 = Mo3N2	9.73	-	-	-
Mo-R069	Mo2 + N2 = 2MoN	14.6	-449.09	-	exergonic
Mo-R070	1/2Mo2 + N2 = MoN2	29.2	-211.5	656.9	exergonic
Mo-R071	30/17Mo2N + N2 = 4/17Mo15N16	7.71	-	-	-
Mo-R072	Mo2N + N2 = Mo2N3	13.61	-	-	-
Mo-R073	6Mo2N + N2 = 4Mo3N2	2.27	-	-	-
Mo-R074	2Mo2N + N2 = 4MoN	6.8	0	-	endergonic

Mo-R075	2/3Mo2N + N2 = 4/3MoN2	20.41	17.4	-	endergonic
Mo-R076	2Mo2N3 + N2 = 4MoN2	5.99	-	-	-
Mo-R077	5/8Mo3H + N2 = 1/8Mo15N16 + 5/16H2	15.17	-	-	-
Mo-R078	4/3Mo3H + N2 = 2Mo2N + 2/3H2	6.92	-600.69	-	exergonic
Mo-R079	4/9Mo3H + N2 = 2/3Mo2N3 + 2/9H2	21.47	-	-	-
Mo-R080	Mo3H + N2 = Mo3N2 + 1/2H2	9.35	-	-	-
Mo-R081	2/3Mo3H + N2 = 2MoN + 1/3H2	14.2	-300.34	-	exergonic
Mo-R082	1/3Mo3H + N2 = MoN2 + 1/6H2	28.75	-137.12	-	exergonic
Mo-R083	6Mo3H + N2 = 18Mo + 2NH3	-0.35	-2060.59	-	exergonic
Mo-R084	30/53Mo3H + N2 = 6/53Mo15N16 + 10/53NH3	15.17	-	-	-
Mo-R085	12/11Mo3H + N2 = 18/11Mo2N + 4/11NH3	6.92	-508.16	-	exergonic
Mo-R086	12/29Mo3H + N2 = 18/29Mo2N3 + 4/29NH3	21.47	-	-	-
Mo-R087	6/7Mo3H + N2 = 6/7Mo3N2 + 2/7NH3	9.35	-	-	-
Mo-R088	3/5Mo3H + N2 = 9/5MoN + 1/5NH3	14.2	-279.49	-	exergonic
Mo-R089	6/19Mo3H + N2 = 18/19MoN2 + 2/19NH3	28.75	-134.74	-	exergonic
Mo-R090	6Mo3H + N2 = 9Mo2 + 2NH3	-0.35	1246.91	416.5	exergonic
Mo-R091	5/3Mo3N2 + N2 = 1/3Mo15N16	5.32	-	-	-
Mo-R092	4/5Mo3N2 + N2 = 6/5Mo2N3	11.09	-	-	-
Mo-R093	2Mo3N2 + N2 = 6MoN	4.43	-	-	-
Mo-R094	1/2Mo3N2 + N2 = 3/2MoN2	17.74	-	-	-
Mo-R095	15/8MoH + N2 = 1/8Mo15N16 + 15/16H2	14.37	-	-	-
Mo-R096	4MoH + N2 = 2Mo2N + 2H2	6.18	-467.29	-	exergonic
Mo-R097	4/3MoH + N2 = 2/3Mo2N3 + 2/3H2	20.63	-	-	-
Mo-R098	3MoH + N2 = Mo3N2 + 3/2H2	8.59	-	-	-
Mo-R099	2MoH + N2 = 2MoN + H2	13.41	-233.64	-	exergonic
Mo-R100	MoH + N2 = MoN2 + 1/2H2	27.85	-103.77	-	exergonic
Mo-R101	6MoH + N2 = 6Mo + 2NH3	-1.04	-547.96	-	exergonic
Mo-R102	9MoH + N2 = 3Mo3H + 2NH3	-0.69	208.35	-	endergonic
Mo-R103	10/7MoH + N2 = 2/21Mo15N16 + 10/21NH3	14.37	-	-	-
Mo-R104	12/5MoH + N2 = 6/5Mo2N + 4/5NH3	6.18	-317.09	-	exergonic
Mo-R105	12/11MoH + N2 = 6/11Mo2N3 + 4/11NH3	20.63	-	-	-
Mo-R106	2MoH + N2 = 2/3Mo3N2 + 2/3NH3	8.59	-	-	-
Mo-R107	3/2MoH + N2 = 3/2MoN + 1/2NH3	13.41	-198.18	-	exergonic
Mo-R108	6/7MoH + N2 = 6/7MoN2 + 2/7NH3	27.85	-102.06	-	exergonic
Mo-R109	6MoH + N2 = 3Mo2 + 2NH3	-1.04	554.54	495.3	exergonic
Mo-R110	30MoN + N2 = 2Mo15N16	0.85	-	-	-
Mo-R111	4MoN + N2 = 2Mo2N3	6.37	-	-	-
Mo-R112	2MoN + N2 = 2MoN2	12.74	26.09	-	endergonic

Table S23: The Ni-based system

ID	**Reaction**	**dm_stoich [%]**	**h298 [kJ/mol]**	**T_eq [°C]**	**Type**
Ni-R001	4Ni + H2 = 2Ni2H	0.86	22.53	-	endergonic
Ni-R002	6Ni + H2 = 2Ni3H	0.57	-	-	-
Ni-R003	2Ni + H2 = 2NiH	1.72	-4.28	-	endergonic
Ni-R004	2/3Ni + H2 = 2/3NiH3	5.15	-	-	-
Ni-R005	4Ni + H2 = 4NiH0.5	0.86	-7.58	-	endergonic

Ni-R006	200/59Ni + H2 = 200/59NiH0.59	1.01	-7.84	-	endergonic
Ni-R007	50/17Ni + H2 = 50/17NiH0.68	1.17	-8.43	-	endergonic
Ni-R008	Ni(H2N)2 + H2 = Ni + 2NH3	-35.32	-	-	-
Ni-R009	4/5Ni(H2N)2 + H2 = 2/5Ni2H + 8/5NH3	-34.76	-	-	-
Ni-R010	6/7Ni(H2N)2 + H2 = 2/7Ni3H + 12/7NH3	-34.95	-	-	-
Ni-R011	2/3Ni(H2N)2 + H2 = 2/3NiH + 4/3NH3	-34.21	-	-	-
Ni-R012	2/5Ni(H2N)2 + H2 = 2/5NiH3 + 4/5NH3	-31.98	-	-	-
Ni-R013	2Ni(H2N)2 + H2 = 2/3Ni3N + 10/3NH3	-30.17	-	-	-
Ni-R014	8/5Ni(H2N)2 + H2 = 2/5Ni4N + 14/5NH3	-31.46	-	-	-
Ni-R015	4/5Ni(H2N)2 + H2 = 4/5NiH0.5 + 8/5NH3	-34.76	-	-	-
Ni-R016	200/259Ni(H2N)2 + H2 = 200/259NiH0.59 + 400/259NH3	-34.66	-	-	-
Ni-R017	50/67Ni(H2N)2 + H2 = 50/67NiH0.68 + 100/67NH3	-34.56	-	-	-
Ni-R018	2Ni2H + H2 = 4NiH	0.85	-31.09	55.9	exergonic
Ni-R019	2/5Ni2H + H2 = 4/5NiH3	4.26	-	-	-
Ni-R020	100/9Ni2H + H2 = 200/9NiH0.59	0.15	-176.57	-	exergonic
Ni-R021	50/9Ni2H + H2 = 100/9NiH0.68	0.31	-94.42	675.3	exergonic
Ni-R022	4Ni3H + H2 = 6Ni2H	0.28	-	-	-
Ni-R023	Ni3H + H2 = 3NiH	1.14	-	-	-
Ni-R024	1/4Ni3H + H2 = 3/4NiH3	4.55	-	-	-
Ni-R025	4Ni3H + H2 = 12NiH0.5	0.28	-	-	-
Ni-R026	200/77Ni3H + H2 = 600/77NiH0.59	0.44	-	-	-
Ni-R027	25/13Ni3H + H2 = 75/13NiH0.68	0.59	-	-	-
Ni-R028	4/3Ni3N + H2 = 2Ni2H + 2/3N2	-6.57	21.41	-	endergonic
Ni-R029	2Ni3N + H2 = 2Ni3H + N2	-6.84	-	-	-
Ni-R030	2/3Ni3N + H2 = 2NiH + 1/3N2	-5.78	-4.84	-	endergonic
Ni-R031	2/9Ni3N + H2 = 2/3NiH3 + 1/9N2	-2.6	-	-	-
Ni-R032	4/3Ni3N + H2 = 4NiH0.5 + 2/3N2	-6.57	-8.7	-	exergonic
Ni-R033	200/177Ni3N + H2 = 200/59NiH0.59 + 100/177N2	-6.43	-8.79	500.5	exergonic
Ni-R034	50/51Ni3N + H2 = 50/17NiH0.68 + 25/51N2	-6.29	-9.25	141.6	exergonic
Ni-R035	2/3Ni3N + H2 = 2Ni + 2/3NH3	-7.37	-31.16	-	exergonic
Ni-R036	4/9Ni3N + H2 = 2/3Ni2H + 4/9NH3	-6.57	-13.26	24.1	exergonic
Ni-R037	1/2Ni3N + H2 = 1/2Ni3H + 1/2NH3	-6.84	-	-	-
Ni-R038	1/3Ni3N + H2 = NiH + 1/3NH3	-5.78	-17.72	37.2	exergonic
Ni-R039	1/6Ni3N + H2 = 1/2NiH3 + 1/6NH3	-2.6	-	-	-
Ni-R040	8/3Ni3N + H2 = 2Ni4N + 2/3NH3	-1.84	-	-	-
Ni-R041	4/9Ni3N + H2 = 4/3NiH0.5 + 4/9NH3	-6.57	-23.3	282.4	exergonic

Ni-R042	200/477Ni3N + H2 = 200/159NiH0.59 + 200/477NH3	-6.43	-22.51	223.7	exergonic
Ni-R043	25/63Ni3N + H2 = 25/21NiH0.68 + 25/63NH3	-6.29	-21.96	174.6	exergonic
Ni-R044	Ni4N + H2 = 2Ni2H + 1/2N2	-4.82	-	-	-
Ni-R045	3/2Ni4N + H2 = 2Ni3H + 3/4N2	-5.09	-	-	-
Ni-R046	1/2Ni4N + H2 = 2NiH + 1/4N2	-4.01	-	-	-
Ni-R047	1/6Ni4N + H2 = 2/3NiH3 + 1/12N2	-0.77	-	-	-
Ni-R048	Ni4N + H2 = 4NiH0.5 + 1/2N2	-4.82	-	-	-
Ni-R049	50/59Ni4N + H2 = 200/59NiH0.59 + 25/59N2	-4.67	-	-	-
Ni-R050	25/34Ni4N + H2 = 50/17NiH0.68 + 25/68N2	-4.53	-	-	-
Ni-R051	2/3Ni4N + H2 = 8/3Ni + 2/3NH3	-5.63	-	-	-
Ni-R052	2/5Ni4N + H2 = 4/5Ni2H + 2/5NH3	-4.82	-	-	-
Ni-R053	6/13Ni4N + H2 = 8/13Ni3H + 6/13NH3	-5.09	-	-	-
Ni-R054	2/7Ni4N + H2 = 8/7NiH + 2/7NH3	-4.01	-	-	-
Ni-R055	2/15Ni4N + H2 = 8/15NiH3 + 2/15NH3	-0.77	-	-	-
Ni-R056	2/5Ni4N + H2 = 8/5NiH0.5 + 2/5NH3	-4.82	-	-	-
Ni-R057	25/67Ni4N + H2 = 100/67NiH0.59 + 25/67NH3	-4.67	-	-	-
Ni-R058	50/143Ni4N + H2 = 200/143NiH0.68 + 50/143NH3	-4.53	-	-	-
Ni-R059	Ni4N3 + H2 = 2Ni2H + 3/2N2	-14.45	-	-	-
Ni-R060	3/2Ni4N3 + H2 = 2Ni3H + 9/4N2	-14.7	-	-	-
Ni-R061	1/2Ni4N3 + H2 = 2NiH + 3/4N2	-13.72	-	-	-
Ni-R062	1/6Ni4N3 + H2 = 2/3NiH3 + 1/4N2	-10.81	-	-	-
Ni-R063	Ni4N3 + H2 = 4NiH0.5 + 3/2N2	-14.45	-	-	-
Ni-R064	50/59Ni4N3 + H2 = 200/59NiH0.59 + 75/59N2	-14.32	-	-	-
Ni-R065	25/34Ni4N3 + H2 = 50/17NiH0.68 + 75/68N2	-14.19	-	-	-
Ni-R066	2/9Ni4N3 + H2 = 8/9Ni + 2/3NH3	-15.18	-	-	-
Ni-R067	2/11Ni4N3 + H2 = 4/11Ni2H + 6/11NH3	-14.45	-	-	-
Ni-R068	6/31Ni4N3 + H2 = 8/31Ni3H + 18/31NH3	-14.7	-	-	-
Ni-R069	2/13Ni4N3 + H2 = 8/13NiH + 6/13NH3	-13.72	-	-	-
Ni-R070	2/21Ni4N3 + H2 = 8/21NiH3 + 2/7NH3	-10.81	-	-	-
Ni-R071	2/5Ni4N3 + H2 = 8/15Ni3N + 2/3NH3	-8.43	-	-	-
Ni-R072	1/3Ni4N3 + H2 = 1/3Ni4N + 2/3NH3	-10.12	-	-	-
Ni-R073	2/11Ni4N3 + H2 = 8/11NiH0.5 + 6/11NH3	-14.45	-	-	-
Ni-R074	25/142Ni4N3 + H2 = 50/71NiH0.59 + 75/142NH3	-14.32	-	-	-
Ni-R075	50/293Ni4N3 + H2 = 200/293NiH0.68 + 150/293NH3	-14.19	-	-	-
Ni-R076	NiH + H2 = NiH3	3.38	-	-	-
Ni-R077	4NiH0.5 + H2 = 4NiH	0.85	-0.98	-	endergonic

Ni-R078	4/5NiH0.5 + H2 = 4/5NiH3	4.26	-	-	-
Ni-R079	200/9NiH0.5 + H2 = 200/9NiH0.59	0.15	-9.31	-	endergonic
Ni-R080	100/9NiH0.5 + H2 = 100/9NiH0.68	0.31	-10.78	-	endergonic
Ni-R081	200/41NiH0.59 + H2 = 200/41NiH	0.7	0.84	-	endergonic
Ni-R082	200/241NiH0.59 + H2 = 200/241NiH3	4.1	-	-	-
Ni-R083	200/9NiH0.59 + H2 = 200/9NiH0.68	0.15	-12.26	-	endergonic
Ni-R084	25/4NiH0.68 + H2 = 25/4NiH	0.54	4.53	-	endergonic
Ni-R085	25/29NiH0.68 + H2 = 25/29NiH3	3.94	-	-	-
Ni-R086	4NiN + H2 = 2Ni2H + 2N2	-18.57	-218.73	-	exergonic
Ni-R087	6NiN + H2 = 2Ni3H + 3N2	-18.8	-	-	-
Ni-R088	2NiN + H2 = 2NiH + N2	-17.88	-124.91	-	exergonic
Ni-R089	2/3NiN + H2 = 2/3NiH3 + 1/3N2	-15.11	-	-	-
Ni-R090	4NiN + H2 = 4NiH0.5 + 2N2	-18.57	-248.84	-	exergonic
Ni-R091	200/59NiN + H2 = 200/59NiH0.59 + 100/59N2	-18.45	-212.3	-	exergonic
Ni-R092	50/17NiN + H2 = 50/17NiH0.68 + 25/17N2	-18.32	-185.83	-	exergonic
Ni-R093	2/3NiN + H2 = 2/3Ni + 2/3NH3	-19.27	-70.81	-	exergonic
Ni-R094	4/7NiN + H2 = 2/7Ni2H + 4/7NH3	-18.57	-57.47	-	exergonic
Ni-R095	3/5NiN + H2 = 1/5Ni3H + 3/5NH3	-18.8	-	-	-
Ni-R096	1/2NiN + H2 = 1/2NiH + 1/2NH3	-17.88	-54.18	-	exergonic
Ni-R097	1/3NiN + H2 = 1/3NiH3 + 1/3NH3	-15.11	-	-	-
Ni-R098	NiN + H2 = 1/3Ni3N + 2/3NH3	-12.84	-90.63	-	exergonic
Ni-R099	8/9NiN + H2 = 2/9Ni4N + 2/3NH3	-14.45	-	-	-
Ni-R100	8/3NiN + H2 = 2/3Ni4N3 + 2/3NH3	-4.82	-	-	-
Ni-R101	4/7NiN + H2 = 4/7NiH0.5 + 4/7NH3	-18.57	-61.78	-	exergonic
Ni-R102	200/359NiN + H2 = 200/359NiH0.59 + 200/359NH3	-18.45	-60.46	-	exergonic
Ni-R103	25/46NiN + H2 = 25/46NiH0.68 + 25/46NH3	-18.32	-59.28	-	exergonic
Ni-R104	6Ni + N2 = 2Ni3N	7.95	1.67	-	endergonic
Ni-R105	8Ni + N2 = 2Ni4N	5.97	-	-	-
Ni-R106	8/3Ni + N2 = 2/3Ni4N3	17.9	-	-	-
Ni-R107	2Ni + N2 = 2NiN	23.86	120.63	-	endergonic
Ni-R108	24Ni(H2N)2 + N2 = 6Ni4N3 + 32NH3	-23.74	-	-	-
Ni-R109	6Ni(H2N)2 + N2 = 6NiN + 8NH3	-19.88	-	-	-
Ni-R110	3Ni2H + N2 = 2Ni3N + 3/2H2	7.04	-32.12	-	exergonic
Ni-R111	4Ni2H + N2 = 2Ni4N + 2H2	5.06	-	-	-
Ni-R112	4/3Ni2H + N2 = 2/3Ni4N3 + 2/3H2	16.89	-	-	-
Ni-R113	Ni2H + N2 = 2NiN + 1/2H2	22.81	109.37	-	endergonic

Ni-R114	6Ni2H + N2 = 12Ni + 2NH3	-0.85	-159.38	-	exergonic
Ni-R115	18Ni2H + N2 = 12Ni3H + 2NH3	-0.28	-	-	-
Ni-R116	2Ni2H + N2 = 4/3Ni3N + 2/3NH3	7.04	-52.01	504.2	exergonic
Ni-R117	12/5Ni2H + N2 = 6/5Ni4N + 4/5NH3	5.06	-	-	-
Ni-R118	12/11Ni2H + N2 = 6/11Ni4N3 + 4/11NH3	16.89	-	-	-
Ni-R119	6/7Ni2H + N2 = 12/7NiN + 2/7NH3	22.81	80.63	-	endergonic
Ni-R120	2Ni3H + N2 = 2Ni3N + H2	7.34	-	-	-
Ni-R121	8/3Ni3H + N2 = 2Ni4N + 4/3H2	5.36	-	-	-
Ni-R122	8/9Ni3H + N2 = 2/3Ni4N3 + 4/9H2	17.23	-	-	-
Ni-R123	2/3Ni3H + N2 = 2NiN + 1/3H2	23.16	-	-	-
Ni-R124	6Ni3H + N2 = 18Ni + 2NH3	-0.57	-	-	-
Ni-R125	3/2Ni3H + N2 = 3/2Ni3N + 1/2NH3	7.34	-	-	-
Ni-R126	24/13Ni3H + N2 = 18/13Ni4N + 8/13NH3	5.36	-	-	-
Ni-R127	24/31Ni3H + N2 = 18/31Ni4N3 + 8/31NH3	17.23	-	-	-
Ni-R128	3/5Ni3H + N2 = 9/5NiN + 1/5NH3	23.16	-	-	-
Ni-R129	8/5Ni3N + N2 = 6/5Ni4N3	9.21	-	-	-
Ni-R130	Ni3N + N2 = 3NiN	14.74	180.11	-	endergonic
Ni-R131	6Ni4N + N2 = 8Ni3N	1.88	-	-	-
Ni-R132	Ni4N + N2 = Ni4N3	11.26	-	-	-
Ni-R133	2/3Ni4N + N2 = 8/3NiN	16.89	-	-	-
Ni-R134	2Ni4N3 + N2 = 8NiN	5.06	-	-	-
Ni-R135	6NiH + N2 = 2Ni3N + 3H2	6.13	14.52	-	exergonic
Ni-R136	8NiH + N2 = 2Ni4N + 4H2	4.18	-	-	-
Ni-R137	8/3NiH + N2 = 2/3Ni4N3 + 4/3H2	15.91	-	-	-
Ni-R138	2NiH + N2 = 2NiN + H2	21.77	124.91	-	endergonic
Ni-R139	6NiH + N2 = 6Ni + 2NH3	-1.69	-78.95	-	exergonic
Ni-R140	12NiH + N2 = 6Ni2H + 2NH3	-0.84	1.49	-	exergonic
Ni-R141	9NiH + N2 = 3Ni3H + 2NH3	-1.13	-	-	-
Ni-R142	3NiH + N2 = Ni3N + NH3	6.13	-38.64	721.7	exergonic
Ni-R143	24/7NiH + N2 = 6/7Ni4N + 8/7NH3	4.18	-	-	-
Ni-R144	24/13NiH + N2 = 6/13Ni4N3 + 8/13NH3	15.91	-	-	-
Ni-R145	3/2NiH + N2 = 3/2NiN + 1/2NH3	21.77	70.74	-	endergonic
Ni-R146	12NiH + N2 = 12NiH0.5 + 2NH3	-0.84	-88.84	-	exergonic
Ni-R147	600/41NiH + N2 = 600/41NiH0.59 + 2NH3	-0.69	-94.32	-	exergonic
Ni-R148	75/4NiH + N2 = 75/4NiH0.68 + 2NH3	-0.54	-105.38	-	exergonic
Ni-R149	6NiH0.5 + N2 = 2Ni3N + 3/2H2	7.04	13.04	-	endergonic

Ni-R150	8NiH0.5 + N2 = 2Ni4N + 2H2	5.06	-	-	-
Ni-R151	8/3NiH0.5 + N2 = 2/3Ni4N3 + 2/3H2	16.89	-	-	-
Ni-R152	2NiH0.5 + N2 = 2NiN + 1/2H2	22.81	124.42	-	endergonic
Ni-R153	12NiH0.5 + N2 = 12Ni + 2NH3	-0.85	-69.05	-	exergonic
Ni-R154	36NiH0.5 + N2 = 12Ni3H + 2NH3	-0.28	-	-	-
Ni-R155	4NiH0.5 + N2 = 4/3Ni3N + 2/3NH3	7.04	-21.9	7.6	exergonic
Ni-R156	24/5NiH0.5 + N2 = 6/5Ni4N + 4/5NH3	5.06	-	-	-
Ni-R157	24/11NiH0.5 + N2 = 6/11Ni4N3 + 4/11NH3	16.89	-	-	-
Ni-R158	12/7NiH0.5 + N2 = 12/7NiN + 2/7NH3	22.81	93.53	-	endergonic
Ni-R159	6NiH0.59 + N2 = 2Ni3N + 177/100H2	6.87	15.56	500.5	exergonic
Ni-R160	8NiH0.59 + N2 = 2Ni4N + 59/25H2	4.9	-	-	-
Ni-R161	8/3NiH0.59 + N2 = 2/3Ni4N3 + 59/75H2	16.72	-	-	-
Ni-R162	2NiH0.59 + N2 = 2NiN + 59/100H2	22.62	125.26	-	endergonic
Ni-R163	600/59NiH0.59 + N2 = 600/59Ni + 2NH3	-1	-68.26	-	exergonic
Ni-R164	200/3NiH0.59 + N2 = 100/3Ni2H + 2NH3	-0.15	437.93	-	endergonic
Ni-R165	1800/77NiH0.59 + N2 = 600/77Ni3H + 2NH3	-0.44	-	-	-
Ni-R166	200/53NiH0.59 + N2 = 200/159Ni3N + 118/159NH3	6.87	-24.28	92.5	exergonic
Ni-R167	300/67NiH0.59 + N2 = 75/67Ni4N + 59/67NH3	4.9	-	-	-
Ni-R168	150/71NiH0.59 + N2 = 75/142Ni4N3 + 59/142NH3	16.72	-	-	-
Ni-R169	600/359NiH0.59 + N2 = 600/359NiN + 118/359NH3	22.62	89.59	-	endergonic
Ni-R170	200/3NiH0.59 + N2 = 200/3NiH0.5 + 2NH3	-0.15	-63.87	-	exergonic
Ni-R171	6NiH0.68 + N2 = 2Ni3N + 51/25H2	6.71	18.87	141.6	exergonic
Ni-R172	8NiH0.68 + N2 = 2Ni4N + 68/25H2	4.74	-	-	-
Ni-R173	8/3NiH0.68 + N2 = 2/3Ni4N3 + 68/75H2	16.54	-	-	-
Ni-R174	2NiH0.68 + N2 = 2NiN + 17/25H2	22.44	126.36	-	endergonic
Ni-R175	150/17NiH0.68 + N2 = 150/17Ni + 2NH3	-1.15	-66.51	-	exergonic
Ni-R176	100/3NiH0.68 + N2 = 50/3Ni2H + 2NH3	-0.31	191.46	-	endergonic
Ni-R177	225/13NiH0.68 + N2 = 75/13Ni3H + 2NH3	-0.59	-	-	-
Ni-R178	25/7NiH0.68 + N2 = 25/21Ni3N + 17/21NH3	6.71	-25.92	206.2	exergonic
Ni-R179	600/143NiH0.68 + N2 = 150/143Ni4N + 136/143NH3	4.74	-	-	-
Ni-R180	600/293NiH0.68 + N2 = 150/293Ni4N3 + 136/293NH3	16.54	-	-	-
Ni-R181	75/46NiH0.68 + N2 = 75/46NiN + 17/46NH3	22.44	86.05	-	endergonic
Ni-R182	100/3NiH0.68 + N2 = 100/3NiH0.5 + 2NH3	-0.31	-59.44	-	exergonic
Ni-R183	200/3NiH0.68 + N2 = 200/3NiH0.59 + 2NH3	-0.15	-55.01	-	exergonic
Ni-R184	6NiH3 + N2 = 2Ni3N + 9H2	2.67	-	-	-
Ni-R185	8NiH3 + N2 = 2Ni4N + 12H2	0.77	-	-	-

Ni-R186	8/3NiH3 + N2 = 2/3Ni4N3 + 4H2	12.12	-	-	-
Ni-R187	2NiH3 + N2 = 2NiN + 3H2	17.8	-	-	-
Ni-R188	2NiH3 + N2 = 2Ni + 2NH3	-4.9	-	-	-
Ni-R189	12/5NiH3 + N2 = 6/5Ni2H + 2NH3	-4.08	-	-	-
Ni-R190	9/4NiH3 + N2 = 3/4Ni3H + 2NH3	-4.36	-	-	-
Ni-R191	3NiH3 + N2 = 3NiH + 2NH3	-3.27	-	-	-
Ni-R192	3/2NiH3 + N2 = 1/2Ni3N + 3/2NH3	2.67	-	-	-
Ni-R193	8/5NiH3 + N2 = 2/5Ni4N + 8/5NH3	0.77	-	-	-
Ni-R194	8/7NiH3 + N2 = 2/7Ni4N3 + 8/7NH3	12.12	-	-	-
Ni-R195	NiH3 + N2 = NiN + NH3	17.8	-	-	-
Ni-R196	12/5NiH3 + N2 = 12/5NiH0.5 + 2NH3	-4.08	-	-	-
Ni-R197	600/241NiH3 + N2 = 600/241NiH0.59 + 2NH3	-3.94	-	-	-
Ni-R198	75/29NiH3 + N2 = 75/29NiH0.68 + 2NH3	-3.79	-	-	-

Table S24: The Sr-based system

ID	**Reaction**	**dm_stoich [%]**	**h298 [kJ/mol]**	**T_eq [°C]**	**Type**
Sr-R001	6Sr + H2 = 2Sr3H	0.38	-	-	-
Sr-R002	Sr + H2 = SrH2	2.3	-180	-	exergonic
Sr-R003	2/3Sr + H2 = 2/3SrH3	3.45	-37.33	99.1	exergonic
Sr-R004	Sr(H2N)2 + H2 = Sr + 2NH3	-26.78	-	-	-
Sr-R005	6/7Sr(H2N)2 + H2 = 2/7Sr3H + 12/7NH3	-26.5	-	-	-
Sr-R006	1/2Sr(H2N)2 + H2 = 1/2SrH2 + NH3	-25.09	-	-	-
Sr-R007	2/5Sr(H2N)2 + H2 = 2/5SrH3 + 4/5NH3	-24.25	-	-	-
Sr-R008	2Sr(H2N)2 + H2 = Sr2HN + 3NH3	-20.51	-	-	-
Sr-R009	4Sr(H2N)2 + H2 = 2Sr2N + 6NH3	-20.93	-	-	-
Sr-R010	2/3Sr2HN + H2 = 4/3SrH2 + 1/3N2	-5.77	-44.91	244.9	exergonic
Sr-R011	2/5Sr2HN + H2 = 4/5SrH3 + 1/5N2	-4.71	72.26	-	endergonic
Sr-R012	Sr2HN + H2 = 2Sr + NH3	-7.89	246.74	-	endergonic
Sr-R013	3/4Sr2HN + H2 = 1/2Sr3H + 3/4NH3	-7.54	-	-	-
Sr-R014	1/3Sr2HN + H2 = 2/3SrH2 + 1/3NH3	-5.77	-37.75	218	exergonic
Sr-R015	1/4Sr2HN + H2 = 1/2SrH3 + 1/4NH3	-4.71	33.69	-	endergonic
Sr-R016	3Sr2N + H2 = 2Sr3H + 3/2N2	-7.05	-	-	-
Sr-R017	1/2Sr2N + H2 = SrH2 + 1/4N2	-5.27	-82.75	523.4	exergonic
Sr-R018	1/3Sr2N + H2 = 2/3SrH3 + 1/6N2	-4.21	27.5	-	endergonic
Sr-R019	2Sr2N + H2 = 2Sr2HN	0.53	-196.29	-	exergonic
Sr-R020	2/3Sr2N + H2 = 4/3Sr + 2/3NH3	-7.4	99.07	-	endergonic
Sr-R021	6/11Sr2N + H2 = 4/11Sr3H + 6/11NH3	-7.05	-	-	-
Sr-R022	2/7Sr2N + H2 = 4/7SrH2 + 2/7NH3	-5.27	-60.4	407.8	exergonic
Sr-R023	2/9Sr2N + H2 = 4/9SrH3 + 2/9NH3	-4.21	8.13	-	endergonic
Sr-R024	2/5Sr3H + H2 = 6/5SrH2	1.91	-	-	-
Sr-R025	1/4Sr3H + H2 = 3/4SrH3	3.06	-	-	-
Sr-R026	2Sr3N2 + H2 = 2Sr3H + 2N2	-9.28	-	-	-
Sr-R027	1/3Sr3N2 + H2 = SrH2 + 1/3N2	-7.55	-49.6	533.1	exergonic

Sr-R028	2/9Sr3N2 + H2 = 2/3SrH3 + 2/9N2	-6.51	49.6	-	endergonic
Sr-R029	4/3Sr3N2 + H2 = 2Sr2HN + 1/3N2	-1.89	-63.67	-	exergonic
Sr-R030	1/3Sr3N2 + H2 = Sr + 2/3NH3	-9.63	99.8	-	endergonic
Sr-R031	2/7Sr3N2 + H2 = 2/7Sr3H + 4/7NH3	-9.28	-	-	-
Sr-R032	1/6Sr3N2 + H2 = 1/2SrH2 + 1/3NH3	-7.55	-40.1	351.5	exergonic
Sr-R033	2/15Sr3N2 + H2 = 2/5SrH3 + 4/15NH3	-6.51	17.52	-	endergonic
Sr-R034	2/3Sr3N2 + H2 = Sr2HN + 1/3NH3	-1.89	-47.13	-	exergonic
Sr-R035	4/3Sr3N2 + H2 = 2Sr2N + 2/3NH3	-2.41	102.02	-	endergonic
Sr-R036	3/2Sr4N3 + H2 = 2Sr3H + 9/4N2	-10.36	-	-	-
Sr-R037	1/4Sr4N3 + H2 = SrH2 + 3/8N2	-8.65	-	-	-
Sr-R038	1/6Sr4N3 + H2 = 2/3SrH3 + 1/4N2	-7.62	-	-	-
Sr-R039	Sr4N3 + H2 = 2Sr2HN + 1/2N2	-3.06	-	-	-
Sr-R040	2/9Sr4N3 + H2 = 8/9Sr + 2/3NH3	-10.71	-	-	-
Sr-R041	6/31Sr4N3 + H2 = 8/31Sr3H + 18/31NH3	-10.36	-	-	-
Sr-R042	2/17Sr4N3 + H2 = 8/17SrH2 + 6/17NH3	-8.65	-	-	-
Sr-R043	2/21Sr4N3 + H2 = 8/21SrH3 + 2/7NH3	-7.62	-	-	-
Sr-R044	2/5Sr4N3 + H2 = 4/5Sr2HN + 2/5NH3	-3.06	-	-	-
Sr-R045	2/3Sr4N3 + H2 = 4/3Sr2N + 2/3NH3	-3.57	-	-	-
Sr-R046	2Sr4N3 + H2 = 8/3Sr3N2 + 2/3NH3	-1.19	-	-	-
Sr-R047	2SrH2 + H2 = 2SrH3	1.12	248.01	-	endergonic
Sr-R048	2SrHN + H2 = 2SrH2 + N2	-12.67	-	-	-
Sr-R049	SrHN + H2 = SrH3 + 1/2N2	-11.68	-	-	-
Sr-R050	SrHN + H2 = Sr + NH3	-14.63	-	-	-
Sr-R051	6/7SrHN + H2 = 2/7Sr3H + 6/7NH3	-14.3	-	-	-
Sr-R052	1/2SrHN + H2 = 1/2SrH2 + 1/2NH3	-12.67	-	-	-
Sr-R053	2/5SrHN + H2 = 2/5SrH3 + 2/5NH3	-11.68	-	-	-
Sr-R054	2SrHN + H2 = Sr2HN + NH3	-7.31	-	-	-
Sr-R055	4SrHN + H2 = 2Sr2N + 2NH3	-7.81	-	-	-
Sr-R056	6SrN + H2 = 2Sr3H + 3N2	-13.45	-	-	-
Sr-R057	SrN + H2 = SrH2 + 1/2N2	-11.8	-50.94	640.5	exergonic
Sr-R058	2/3SrN + H2 = 2/3SrH3 + 1/3N2	-10.81	48.71	-	endergonic
Sr-R059	4SrN + H2 = 2Sr2HN + N2	-6.4	-69.05	-	exergonic
Sr-R060	2SrN + H2 = 2SrHN	0.99	-	-	-
Sr-R061	2/3SrN + H2 = 2/3Sr + 2/3NH3	-13.78	55.44	-	endergonic
Sr-R062	3/5SrN + H2 = 1/5Sr3H + 3/5NH3	-13.45	-	-	-
Sr-R063	2/5SrN + H2 = 2/5SrH2 + 2/5NH3	-11.8	-38.73	346.4	exergonic
Sr-R064	1/3SrN + H2 = 1/3SrH3 + 1/3NH3	-10.81	9.06	-	endergonic
Sr-R065	SrN + H2 = 1/2Sr2HN + 1/2NH3	-6.4	-40.21	716.8	exergonic
Sr-R066	4/3SrN + H2 = 2/3Sr2N + 2/3NH3	-6.89	11.82	-	endergonic
Sr-R067	2SrN + H2 = 2/3Sr3N2 + 2/3NH3	-4.59	-33.29	322.9	exergonic
Sr-R068	8/3SrN + H2 = 2/3Sr4N3 + 2/3NH3	-3.45	-	-	-
Sr-R069	6SrN2 + H2 = 2Sr3H + 6N2	-23.94	-	-	-
Sr-R070	SrN2 + H2 = SrH2 + N2	-22.48	0.39	-	exergonic
Sr-R071	2/3SrN2 + H2 = 2/3SrH3 + 2/3N2	-21.61	82.93	-	endergonic
Sr-R072	1/2SrN2 + H2 = 1/2Sr(H2N)2	3.49	-	-	-
Sr-R073	4SrN2 + H2 = 2Sr2HN + 3N2	-17.73	136.29	99.7	exergonic
Sr-R074	2SrN2 + H2 = 2SrHN + N2	-11.24	-	-	-
Sr-R075	1/3SrN2 + H2 = 1/3Sr + 2/3NH3	-24.23	29.53	-	endergonic
Sr-R076	6/19SrN2 + H2 = 2/19Sr3H + 12/19NH3	-23.94	-	-	-

Sr-R077	1/4SrN2 + H2 = 1/4SrH2 + 1/2NH3	-22.48	-22.85	241.3	exergonic
Sr-R078	2/9SrN2 + H2 = 2/9SrH3 + 4/9NH3	-21.61	7.25	-	endergonic
Sr-R079	2/5SrN2 + H2 = 1/5Sr2HN + 3/5NH3	-17.73	-13.91	278.6	exergonic
Sr-R080	1/2SrN2 + H2 = 1/2SrHN + 1/2NH3	-11.24	-	-	-
Sr-R081	4/9SrN2 + H2 = 2/9Sr2N + 2/3NH3	-18.17	6.36	-	endergonic
Sr-R082	1/2SrN2 + H2 = 1/6Sr3N2 + 2/3NH3	-16.15	-5.6	-	endergonic
Sr-R083	8/15SrN2 + H2 = 2/15Sr4N3 + 2/3NH3	-15.14	-	-	-
Sr-R084	2/3SrN2 + H2 = 2/3SrN + 2/3NH3	-12.11	3.63	-	endergonic
Sr-R085	6SrN6 + H2 = 2Sr3H + 18N2	-48.76	-	-	-
Sr-R086	SrN6 + H2 = SrH2 + 3N2	-47.78	-	-	-
Sr-R087	2/3SrN6 + H2 = 2/3SrH3 + 2N2	-47.2	-	-	-
Sr-R088	1/2SrN6 + H2 = 1/2Sr(H2N)2 + N2	-30.29	-	-	-
Sr-R089	4SrN6 + H2 = 2Sr2HN + 11N2	-44.58	-	-	-
Sr-R090	2SrN6 + H2 = 2SrHN + 5N2	-40.21	-	-	-
Sr-R091	1/9SrN6 + H2 = 1/9Sr + 2/3NH3	-48.96	-	-	-
Sr-R092	6/55SrN6 + H2 = 2/55Sr3H + 36/55NH3	-48.76	-	-	-
Sr-R093	1/10SrN6 + H2 = 1/10SrH2 + 3/5NH3	-47.78	-	-	-
Sr-R094	2/21SrN6 + H2 = 2/21SrH3 + 4/7NH3	-47.2	-	-	-
Sr-R095	1/8SrN6 + H2 = 1/8Sr(H2N)2 + 1/2NH3	-30.29	-	-	-
Sr-R096	2/17SrN6 + H2 = 1/17Sr2HN + 11/17NH3	-44.58	-	-	-
Sr-R097	1/8SrN6 + H2 = 1/8SrHN + 5/8NH3	-40.21	-	-	-
Sr-R098	4/33SrN6 + H2 = 2/33Sr2N + 2/3NH3	-44.88	-	-	-
Sr-R099	1/8SrN6 + H2 = 1/24Sr3N2 + 2/3NH3	-43.52	-	-	-
Sr-R100	8/63SrN6 + H2 = 2/63Sr4N3 + 2/3NH3	-42.84	-	-	-
Sr-R101	2/15SrN6 + H2 = 2/15SrN + 2/3NH3	-40.8	-	-	-
Sr-R102	1/6SrN6 + H2 = 1/6SrN2 + 2/3NH3	-32.64	-	-	-
Sr-R103	4Sr + N2 = 2Sr2N	7.99	-388.99	-	exergonic
Sr-R104	3Sr + N2 = Sr3N2	10.66	-391.21	-	exergonic
Sr-R105	8/3Sr + N2 = 2/3Sr4N3	11.99	-	-	-
Sr-R106	2Sr + N2 = 2SrN	15.99	-258.12	-	exergonic
Sr-R107	Sr + N2 = SrN2	31.97	-180.39	-	exergonic
Sr-R108	1/3Sr + N2 = 1/3SrN6	95.92	-	-	-
Sr-R109	1/2Sr(H2N)2 + N2 = 1/2SrN6 + H2	43.45	-	-	-
Sr-R110	24Sr(H2N)2 + N2 = 6Sr4N3 + 32NH3	-18	-	-	-
Sr-R111	6Sr(H2N)2 + N2 = 6SrN + 8NH3	-15.07	-	-	-
Sr-R112	3/2Sr(H2N)2 + N2 = 3/2SrN2 + 2NH3	-3.37	-	-	-
Sr-R113	3/8Sr(H2N)2 + N2 = 3/8SrN6 + 1/2NH3	43.45	-	-	-
Sr-R114	6Sr2HN + N2 = 4Sr3N2 + 3H2	1.92	191.01	-	endergonic
Sr-R115	4Sr2HN + N2 = 2Sr4N3 + 2H2	3.15	-	-	-
Sr-R116	2Sr2HN + N2 = 4SrN + H2	6.83	69.05	-	endergonic
Sr-R117	2/3Sr2HN + N2 = 4/3SrN2 + 1/3H2	21.56	-45.43	99.7	exergonic
Sr-R118	2/11Sr2HN + N2 = 4/11SrN6 + 1/11H2	80.45	-	-	-
Sr-R119	6Sr2HN + N2 = 6Sr2N + 2NH3	-0.53	497.08	-	endergonic
Sr-R120	3Sr2HN + N2 = 2Sr3N2 + NH3	1.92	49.61	-	endergonic
Sr-R121	12/5Sr2HN + N2 = 6/5Sr4N3 + 4/5NH3	3.15	-	-	-
Sr-R122	3/2Sr2HN + N2 = 3SrN + 1/2NH3	6.83	28.84	-	endergonic
Sr-R123	3/5Sr2HN + N2 = 6/5SrN2 + 1/5NH3	21.56	-50.07	113.3	exergonic
Sr-R124	3/17Sr2HN + N2 = 6/17SrN6 + 1/17NH3	80.45	-	-	-
Sr-R125	6Sr2N + N2 = 4Sr3N2	2.47	-397.86	506.1	exergonic

Sr-R126	4Sr2N + N2 = 2Sr4N3	3.7	-	-	-
Sr-R127	2Sr2N + N2 = 4SrN	7.4	-127.24	368.5	exergonic
Sr-R128	2/3Sr2N + N2 = 4/3SrN2	22.2	-110.86	387.7	exergonic
Sr-R129	2/11Sr2N + N2 = 4/11SrN6	81.42	-	-	-
Sr-R130	4/3Sr3H + N2 = 2Sr2N + 2/3H2	7.58	-	-	-
Sr-R131	Sr3H + N2 = Sr3N2 + 1/2H2	10.23	-	-	-
Sr-R132	8/9Sr3H + N2 = 2/3Sr4N3 + 4/9H2	11.56	-	-	-
Sr-R133	2/3Sr3H + N2 = 2SrN + 1/3H2	15.54	-	-	-
Sr-R134	1/3Sr3H + N2 = SrN2 + 1/6H2	31.47	-	-	-
Sr-R135	1/9Sr3H + N2 = 1/3SrN6 + 1/18H2	95.17	-	-	-
Sr-R136	6Sr3H + N2 = 18Sr + 2NH3	-0.38	-	-	-
Sr-R137	12/11Sr3H + N2 = 18/11Sr2N + 4/11NH3	7.58	-	-	-
Sr-R138	6/7Sr3H + N2 = 6/7Sr3N2 + 2/7NH3	10.23	-	-	-
Sr-R139	24/31Sr3H + N2 = 18/31Sr4N3 + 8/31NH3	11.56	-	-	-
Sr-R140	3/5Sr3H + N2 = 9/5SrN + 1/5NH3	15.54	-	-	-
Sr-R141	6/19Sr3H + N2 = 18/19SrN2 + 2/19NH3	31.47	-	-	-
Sr-R142	6/55Sr3H + N2 = 18/55SrN6 + 2/55NH3	95.17	-	-	-
Sr-R143	8Sr3N2 + N2 = 6Sr4N3	1.2	-	-	-
Sr-R144	2Sr3N2 + N2 = 6SrN	4.82	8.07	-	endergonic
Sr-R145	1/2Sr3N2 + N2 = 3/2SrN2	19.26	-74.99	328.3	exergonic
Sr-R146	1/8Sr3N2 + N2 = 3/8SrN6	77.05	-	-	-
Sr-R147	2Sr4N3 + N2 = 8SrN	3.57	-	-	-
Sr-R148	2/5Sr4N3 + N2 = 8/5SrN2	17.84	-	-	-
Sr-R149	2/21Sr4N3 + N2 = 8/21SrN6	74.94	-	-	-
Sr-R150	4SrH2 + N2 = 2Sr2HN + 3H2	6.13	134.72	244.9	exergonic
Sr-R151	2SrH2 + N2 = 2SrHN + H2	14.5	-	-	-
Sr-R152	4SrH2 + N2 = 2Sr2N + 4H2	5.56	331.01	523.4	exergonic
Sr-R153	3SrH2 + N2 = Sr3N2 + 3H2	8.17	148.79	533.1	exergonic
Sr-R154	8/3SrH2 + N2 = 2/3Sr4N3 + 8/3H2	9.47	-	-	-
Sr-R155	2SrH2 + N2 = 2SrN + 2H2	13.38	101.88	640.5	exergonic
Sr-R156	SrH2 + N2 = SrN2 + H2	29	-0.39	-	endergonic
Sr-R157	1/3SrH2 + N2 = 1/3SrN6 + 1/3H2	91.51	-	-	-
Sr-R158	3SrH2 + N2 = 3Sr + 2NH3	-2.25	448.2	-	endergonic
Sr-R159	18/5SrH2 + N2 = 6/5Sr3H + 2NH3	-1.87	-	-	-
Sr-R160	2SrH2 + N2 = Sr2HN + NH3	6.13	21.46	442.9	exergonic
Sr-R161	3/2SrH2 + N2 = 3/2SrHN + 1/2NH3	14.5	-	-	-
Sr-R162	12/7SrH2 + N2 = 6/7Sr2N + 8/7NH3	5.56	89.41	-	endergonic
Sr-R163	3/2SrH2 + N2 = 1/2Sr3N2 + NH3	8.17	28.5	-	endergonic
Sr-R164	24/17SrH2 + N2 = 6/17Sr4N3 + 16/17NH3	9.47	-	-	-
Sr-R165	6/5SrH2 + N2 = 6/5SrN + 4/5NH3	13.38	24.41	-	endergonic
Sr-R166	3/4SrH2 + N2 = 3/4SrN2 + 1/2NH3	29	-23.24	54.3	exergonic
Sr-R167	3/10SrH2 + N2 = 3/10SrN6 + 1/5NH3	91.51	-	-	-
Sr-R168	4SrH3 + N2 = 2Sr2HN + 5H2	4.95	-361.3	-	exergonic
Sr-R169	2SrH3 + N2 = 2SrHN + 2H2	13.23	-	-	-
Sr-R170	4SrH3 + N2 = 2Sr2N + 6H2	4.39	-165	-	exergonic
Sr-R171	3SrH3 + N2 = Sr3N2 + 9/2H2	6.97	-223.22	-	exergonic
Sr-R172	8/3SrH3 + N2 = 2/3Sr4N3 + 4H2	8.25	-	-	-
Sr-R173	2SrH3 + N2 = 2SrN + 3H2	12.12	-146.12	-	exergonic
Sr-R174	SrH3 + N2 = SrN2 + 3/2H2	27.57	-124.4	-	exergonic

Sr-R175	1/3SrH3 + N2 = 1/3SrN6 + 1/2H2	89.38	-	-	-
Sr-R176	2SrH3 + N2 = 2Sr + 2NH3	-3.34	20.2	-	exergonic
Sr-R177	9/4SrH3 + N2 = 3/4Sr3H + 2NH3	-2.97	-	-	-
Sr-R178	6SrH3 + N2 = 6SrH2 + 2NH3	-1.11	-835.81	-	exergonic
Sr-R179	3/2SrH3 + N2 = 3/4Sr2HN + 5/4NH3	4.95	-192.86	-	exergonic
Sr-R180	6/5SrH3 + N2 = 6/5SrHN + 4/5NH3	13.23	-	-	-
Sr-R181	4/3SrH3 + N2 = 2/3Sr2N + 4/3NH3	4.39	-116.2	-	exergonic
Sr-R182	6/5SrH3 + N2 = 2/5Sr3N2 + 6/5NH3	6.97	-144.36	-	exergonic
Sr-R183	8/7SrH3 + N2 = 2/7Sr4N3 + 8/7NH3	8.25	-	-	-
Sr-R184	SrH3 + N2 = SrN + NH3	12.12	-118.96	-	exergonic
Sr-R185	2/3SrH3 + N2 = 2/3SrN2 + 2/3NH3	27.57	-113.53	-	exergonic
Sr-R186	2/7SrH3 + N2 = 2/7SrN6 + 2/7NH3	89.38	-	-	-
Sr-R187	2SrHN + N2 = 2SrN2 + H2	12.67	-	-	-
Sr-R188	2/5SrHN + N2 = 2/5SrN6 + 1/5H2	67.25	-	-	-
Sr-R189	24SrHN + N2 = 6Sr4N3 + 8NH3	-4.39	-	-	-
Sr-R190	6SrHN + N2 = 6SrN + 2NH3	-0.98	-	-	-
Sr-R191	3/2SrHN + N2 = 3/2SrN2 + 1/2NH3	12.67	-	-	-
Sr-R192	3/8SrHN + N2 = 3/8SrN6 + 1/8NH3	67.25	-	-	-
Sr-R193	2SrN + N2 = 2SrN2	13.78	-102.67	400.4	exergonic
Sr-R194	2/5SrN + N2 = 2/5SrN6	68.91	-	-	-
Sr-R195	1/2SrN2 + N2 = 1/2SrN6	48.45	-	-	-

Table S25: The W-based system

ID	**Reaction**	**dm_stoich [%]**	**h298 [kJ/mol]**	**T_eq [°C]**	**Type**
W-R01	2/3W2N + H2 = 4/3W + 2/3NH3	-3.67	64.06	-	endergonic
W-R02	2/9W2N3 + H2 = 4/9W + 2/3NH3	-10.26	-	-	-
W-R03	1/3W2N3 + H2 = 1/3W2N + 2/3NH3	-6.84	-	-	-
W-R04	2W2N3 + H2 = 4/3W3N4 + 2/3NH3	-1.14	-	-	-
W-R05	14/27W2N3 + H2 = 4/27W7N6 + 2/3NH3	-4.4	-	-	-
W-R06	2/3W2N3 + H2 = 4/3WN + 2/3NH3	-3.42	-	-	-
W-R07	1/6W3N4 + H2 = 1/2W + 2/3NH3	-9.22	-11.95	240.2	exergonic
W-R08	4/15W3N4 + H2 = 2/5W2N + 2/3NH3	-5.76	-57.55	-	exergonic
W-R09	7/15W3N4 + H2 = 1/5W7N6 + 2/3NH3	-3.29	-	-	-
W-R10	2/3W3N4 + H2 = 2WN + 2/3NH3	-2.31	-23.97	164.7	exergonic
W-R11	1/9W7N6 + H2 = 7/9W + 2/3NH3	-6.13	-	-	-
W-R12	4/15W7N6 + H2 = 14/15W2N + 2/3NH3	-2.55	-	-	-
W-R13	2/3WN + H2 = 2/3W + 2/3NH3	-7.08	-7.94	318.2	exergonic
W-R14	4/3WN + H2 = 2/3W2N + 2/3NH3	-3.54	-79.94	-	exergonic
W-R15	14/3WN + H2 = 2/3W7N6 + 2/3NH3	-1.01	-	-	-
W-R16	1/27WN18 + H2 = 1/27W + 2/3NH3	-57.83	-	-	-
W-R17	4/105WN18 + H2 = 2/105W2N + 2/3NH3	-56.23	-	-	-
W-	4/99WN18 + H2 = 2/99W2N3 + 2/3NH3	-53.01	-	-	-

R18					
W-R19	1/25WN18 + H2 = 1/75W3N4 + 2/3NH3	-53.55	-	-	-
W-R20	7/180WN18 + H2 = 1/180W7N6 + 2/3NH3	-55.08	-	-	-
W-R21	2/51WN18 + H2 = 2/51WN + 2/3NH3	-54.62	-	-	-
W-R22	1/24WN18 + H2 = 1/24WN2 + 2/3NH3	-51.41	-	-	-
W-R23	1/18WN18 + H2 = 1/18WN6 + 2/3NH3	-38.55	-	-	-
W-R24	1/3WN2 + H2 = 1/3W + 2/3NH3	-13.22	8.12	-	endergonic
W-R25	4/9WN2 + H2 = 2/9W2N + 2/3NH3	-9.92	-10.53	103.7	exergonic
W-R26	4/3WN2 + H2 = 2/3W2N3 + 2/3NH3	-3.31	-	-	-
W-R27	WN2 + H2 = 1/3W3N4 + 2/3NH3	-4.41	48.25	-	endergonic
W-R28	7/12WN2 + H2 = 1/12W7N6 + 2/3NH3	-7.56	-	-	-
W-R29	2/3WN2 + H2 = 2/3WN + 2/3NH3	-6.61	24.17	-	endergonic
W-R30	1/9WN6 + H2 = 1/9W + 2/3NH3	-31.37	-	-	-
W-R31	4/33WN6 + H2 = 2/33W2N + 2/3NH3	-28.76	-	-	-
W-R32	4/27WN6 + H2 = 2/27W2N3 + 2/3NH3	-23.53	-	-	-
W-R33	1/7WN6 + H2 = 1/21W3N4 + 2/3NH3	-24.4	-	-	-
W-R34	7/54WN6 + H2 = 1/54W7N6 + 2/3NH3	-26.89	-	-	-
W-R35	2/15WN6 + H2 = 2/15WN + 2/3NH3	-26.14	-	-	-
W-R36	1/6WN6 + H2 = 1/6WN2 + 2/3NH3	-20.92	-	-	-
W-R37	4W + N2 = 2W2N	3.81	-283.98	-	exergonic
W-R38	4/3W + N2 = 2/3W2N3	11.43	-	-	-
W-R39	3/2W + N2 = 1/2W3N4	10.16	-55.95	142.3	exergonic
W-R40	7/3W + N2 = 1/3W7N6	6.53	-	-	-
W-R41	2W + N2 = 2WN	7.62	-67.97	133.2	exergonic
W-R42	1/9W + N2 = 1/9WN18	137.14	-	-	-
W-R43	W + N2 = WN2	15.24	-116.14	-	exergonic
W-R44	1/3W + N2 = 1/3WN6	45.71	-	-	-
W-R45	W2N + N2 = W2N3	7.34	-	-	-
W-R46	6/5W2N + N2 = 4/5W3N4	6.12	80.87	-	endergonic
W-R47	14/5W2N + N2 = 4/5W7N6	2.62	-	-	-
W-R48	2W2N + N2 = 4WN	3.67	148.03	-	endergonic
W-R49	2/35W2N + N2 = 4/35WN18	128.44	-	-	-
W-R50	2/3W2N + N2 = 4/3WN2	11.01	-60.2	298.1	exergonic
W-R51	2/11W2N + N2 = 4/11WN6	40.37	-	-	-
W-R52	2/33W2N3 + N2 = 4/33WN18	112.82	-	-	-
W-R53	2W2N3 + N2 = 4WN2	3.42	-	-	-

W-R54	2/9W2N3 + N2 = 4/9WN6	30.77	-	-	-
W-R55	4W3N4 + N2 = 6W2N3	1.15	-	-	-
W-R56	1/25W3N4 + N2 = 3/25WN18	115.27	-	-	-
W-R57	W3N4 + N2 = 3WN2	4.61	-236.53	-	exergonic
W-R58	1/7W3N4 + N2 = 3/7WN6	32.28	-	-	-
W-R59	4/9W7N6 + N2 = 14/9W2N3	4.6	-	-	-
W-R60	3/5W7N6 + N2 = 7/5W3N4	3.41	-	-	-
W-R61	2W7N6 + N2 = 14WN	1.02	-	-	-
W-R62	1/60W7N6 + N2 = 7/60WN18	122.61	-	-	-
W-R63	1/4W7N6 + N2 = 7/4WN2	8.17	-	-	-
W-R64	1/18W7N6 + N2 = 7/18WN6	36.78	-	-	-
W-R65	4WN + N2 = 2W2N3	3.54	-	-	-
W-R66	6WN + N2 = 2W3N4	2.36	-19.88	338.5	exergonic
W-R67	2/17WN + N2 = 2/17WN18	120.36	-	-	-
W-R68	2WN + N2 = 2WN2	7.08	-164.31	-	exergonic
W-R69	2/5WN + N2 = 2/5WN6	35.4	-	-	-
W-R70	1/8WN2 + N2 = 1/8WN18	105.79	-	-	-
W-R71	1/2WN2 + N2 = 1/2WN6	26.45	-	-	-
W-R72	1/6WN6 + N2 = 1/6WN18	62.75	-	-	-

Table S26: The Zn-based system

ID	**Reaction**	**dm_stoich [%]**	**h298 [kJ/mol]**	**T_eq [°C]**	**Type**
Zn-R01	2Zn + H2 = 2ZnH	1.54	-	-	-
Zn-R02	1/3Zn + H2 = 1/3ZnH6	9.25	-	-	-
Zn-R03	1/9Zn(H15N8)2 + H2 = 1/9Zn + 16/9NH3	-79.55	-	-	-
Zn-R04	2/19Zn(H15N8)2 + H2 = 2/19ZnH + 32/19NH3	-79.24	-	-	-
Zn-R05	1/12Zn(H15N8)2 + H2 = 1/12ZnH6 + 4/3NH3	-77.66	-	-	-
Zn-R06	1/8Zn(H15N8)2 + H2 = 1/8Zn(H2N)2 + 7/4NH3	-69.53	-	-	-
Zn-R07	2/17Zn(H15N8)2 + H2 = 2/51Zn3N + 94/51NH3	-78.09	-	-	-
Zn-R08	1/8Zn(H15N8)2 + H2 = 1/24Zn3N2 + 23/12NH3	-76.63	-	-	-
Zn-R09	2/15Zn(H15N8)2 + H2 = 2/15ZnN + 2NH3	-75.17	-	-	-
Zn-R10	Improbable stoichiometric coefficients	-53.27	-	-	-
Zn-R11	Zn(H2N)2 + H2 = ZnH6 + N2	-26.68	-	-	-
Zn-R12	Zn(H2N)2 + H2 = Zn + 2NH3	-32.89	-	-	-
Zn-R13	2/3Zn(H2N)2 + H2 = 2/3ZnH + 4/3NH3	-31.86	-	-	-
Zn-R14	1/4Zn(H2N)2 + H2 = 1/4ZnH6 + 1/2NH3	-26.68	-	-	-

Zn-R15	2Zn(H2N)2 + H2 = 2/3Zn3N + 10/3NH3	-28.1	-	-	-
Zn-R16	1/11Zn(H4N5)2 + H2 = 1/11Zn + 10/11NH3	-69.38	-	-	-
Zn-R17	2/23Zn(H4N5)2 + H2 = 2/23ZnH + 20/23NH3	-68.91	-	-	-
Zn-R18	1/14Zn(H4N5)2 + H2 = 1/14ZnH6 + 5/7NH3	-66.55	-	-	-
Zn-R19	1/10Zn(H4N5)2 + H2 = 1/10Zn(H2N)2 + 4/5NH3	-54.37	-	-	-
Zn-R20	2/21Zn(H4N5)2 + H2 = 2/63Zn3N + 58/63NH3	-67.19	-	-	-
Zn-R21	1/10Zn(H4N5)2 + H2 = 1/30Zn3N2 + 14/15NH3	-65.01	-	-	-
Zn-R22	2/19Zn(H4N5)2 + H2 = 2/19ZnN + 18/19NH3	-62.82	-	-	-
Zn-R23	1/2Zn(H4N5)2 + H2 = 1/2ZnN6 + 2NH3	-30.02	-	-	-
Zn-R24	2/3Zn3N + H2 = 2ZnH + 1/3N2	-5.23	-	-	-
Zn-R25	1/9Zn3N + H2 = 1/3ZnH6 + 1/18N2	1.97	-	-	-
Zn-R26	2/3Zn3N + H2 = 2Zn + 2/3NH3	-6.67	-	-	-
Zn-R27	1/3Zn3N + H2 = ZnH + 1/3NH3	-5.23	-	-	-
Zn-R28	2/21Zn3N + H2 = 2/7ZnH6 + 2/21NH3	1.97	-	-	-
Zn-R29	2/3Zn3N2 + H2 = 2ZnH + 2/3N2	-11.15	-	-	-
Zn-R30	1/9Zn3N2 + H2 = 1/3ZnH6 + 1/9N2	-4.4	-	-	-
Zn-R31	1/3Zn3N2 + H2 = Zn + 2/3NH3	-12.5	-23.21	-	exergonic
Zn-R32	2/9Zn3N2 + H2 = 2/3ZnH + 4/9NH3	-11.15	-	-	-
Zn-R33	1/12Zn3N2 + H2 = 1/4ZnH6 + 1/6NH3	-4.4	-	-	-
Zn-R34	2/3Zn3N2 + H2 = 2/3Zn3N + 2/3NH3	-6.25	-	-	-
Zn-R35	2/5ZnH + H2 = 2/5ZnH6	7.59	-	-	-
Zn-R36	2ZnN + H2 = 2ZnH + N2	-16.37	-	-	-
Zn-R37	1/3ZnN + H2 = 1/3ZnH6 + 1/6N2	-10.03	-	-	-
Zn-R38	2/3ZnN + H2 = 2/3Zn + 2/3NH3	-17.64	-97.49	-	exergonic
Zn-R39	1/2ZnN + H2 = 1/2ZnH + 1/2NH3	-16.37	-	-	-
Zn-R40	2/9ZnN + H2 = 2/9ZnH6 + 2/9NH3	-10.03	-	-	-
Zn-R41	ZnN + H2 = 1/3Zn3N + 2/3NH3	-11.76	-	-	-
Zn-R42	2ZnN + H2 = 2/3Zn3N2 + 2/3NH3	-5.88	-246.07	-	exergonic
Zn-R43	2ZnN6 + H2 = 2ZnH + 6N2	-55.57	-	-	-
Zn-R44	1/3ZnN6 + H2 = 1/3ZnH6 + N2	-52.2	-	-	-
Zn-R45	1/2ZnN6 + H2 = 1/2Zn(H2N)2 + N2	-34.8	-	-	-
Zn-R46	1/9ZnN6 + H2 = 1/9Zn + 2/3NH3	-56.24	-	-	-
Zn-R47	2/19ZnN6 + H2 = 2/19ZnH + 12/19NH3	-55.57	-	-	-
Zn-R48	1/12ZnN6 + H2 = 1/12ZnH6 + 1/2NH3	-52.2	-	-	-
Zn-R49	1/8ZnN6 + H2 = 1/8Zn(H2N)2 + 1/2NH3	-34.8	-	-	-
Zn-R50	2/17ZnN6 + H2 = 2/51Zn3N + 2/3NH3	-53.12	-	-	-

Zn-R51	1/8ZnN6 + H2 = 1/24Zn3N2 + 2/3NH3	-50	-	-	-
Zn-R52	2/15ZnN6 + H2 = 2/15ZnN + 2/3NH3	-46.87	-	-	-
Zn-R53	6Zn + N2 = 2Zn3N	7.14	-	-	-
Zn-R54	3Zn + N2 = Zn3N2	14.28	-22.17	-	endergonic
Zn-R55	2Zn + N2 = 2ZnN	21.42	200.69	-	endergonic
Zn-R56	1/3Zn + N2 = 1/3ZnN6	128.54	-	-	-
Zn-R57	3/2Zn(H15N8)2 + N2 = 3/2Zn(H4N5)2 + 11NH3	-33.22	-	-	-
Zn-R58	1/2Zn(H2N)2 + N2 = 1/2ZnN6 + H2	53.37	-	-	-
Zn-R59	6Zn(H2N)2 + N2 = 6ZnN + 8NH3	-18.52	-	-	-
Zn-R60	3/8Zn(H2N)2 + N2 = 3/8ZnN6 + 1/2NH3	53.37	-	-	-
Zn-R61	2Zn3N + N2 = 2Zn3N2	6.67	-	-	-
Zn-R62	Zn3N + N2 = 3ZnN	13.33	-	-	-
Zn-R63	2/17Zn3N + N2 = 6/17ZnN6	113.31	-	-	-
Zn-R64	2Zn3N2 + N2 = 6ZnN	6.25	646.42	-	endergonic
Zn-R65	1/8Zn3N2 + N2 = 3/8ZnN6	99.98	-	-	-
Zn-R66	6ZnH + N2 = 2Zn3N + 3H2	5.51	-	-	-
Zn-R67	3ZnH + N2 = Zn3N2 + 3/2H2	12.55	-	-	-
Zn-R68	2ZnH + N2 = 2ZnN + H2	19.58	-	-	-
Zn-R69	1/3ZnH + N2 = 1/3ZnN6 + 1/6H2	125.07	-	-	-
Zn-R70	6ZnH + N2 = 6Zn + 2NH3	-1.52	-	-	-
Zn-R71	3ZnH + N2 = Zn3N + NH3	5.51	-	-	-
Zn-R72	2ZnH + N2 = 2/3Zn3N2 + 2/3NH3	12.55	-	-	-
Zn-R73	3/2ZnH + N2 = 3/2ZnN + 1/2NH3	19.58	-	-	-
Zn-R74	6/19ZnH + N2 = 6/19ZnN6 + 2/19NH3	125.07	-	-	-
Zn-R75	ZnH6 + N2 = Zn(H2N)2 + H2	36.4	-	-	-
Zn-R76	6ZnH6 + N2 = 2Zn3N + 18H2	-1.93	-	-	-
Zn-R77	3ZnH6 + N2 = Zn3N2 + 9H2	4.61	-	-	-
Zn-R78	2ZnH6 + N2 = 2ZnN + 6H2	11.14	-	-	-
Zn-R79	1/3ZnH6 + N2 = 1/3ZnN6 + H2	109.19	-	-	-
Zn-R80	ZnH6 + N2 = Zn + 2NH3	-8.47	-	-	-
Zn-R81	6/5ZnH6 + N2 = 6/5ZnH + 2NH3	-7.06	-	-	-
Zn-R82	3/4ZnH6 + N2 = 3/4Zn(H2N)2 + 1/2NH3	36.4	-	-	-
Zn-R83	6/7ZnH6 + N2 = 2/7Zn3N + 12/7NH3	-1.93	-	-	-
Zn-R84	3/4ZnH6 + N2 = 1/4Zn3N2 + 3/2NH3	4.61	-	-	-
Zn-R85	2/3ZnH6 + N2 = 2/3ZnN + 4/3NH3	11.14	-	-	-
Zn-R86	1/4ZnH6 + N2 = 1/4ZnN6 + 1/2NH3	109.19	-	-	-

Zn-R87	2/5ZnN + N2 = 2/5ZnN6	88.22	-	-	-

1.5 Nitridation and hydrogenation reactions for the ideal cycle II

Table S27: Nitridation reactions examined in the Ellingham diagram of Figure 2a.

ID	Reaction	dm_stoich [%]	h298 [kJ/mol]	T_eq [°C]	Type
Al-R20	2Al + N2 = 2AlN	51.91	-635.97	-	exergonic
Ca-R125	4Ca + N2 = 2Ca2N	17.47	-519.68	-	exergonic
Co-R081	6Co + N2 = 2Co3N	7.92	16.74	-	endergonic
Cr-R066	4Cr + N2 = 2Cr2N	13.47	-251.04	-	exergonic
Cu-R48	2/3Cu + N2 = 2/3CuN3	66.13	75.6	-	endergonic
Fe-R131	6Fe + N2 = 2Fe3N	8.36	-121.76	218.7	exergonic
Li-R102	6Li + N2 = 2Li3N	67.28	-329.11	-	exergonic
Mn-R52	8Mn + N2 = 2Mn4N	6.37	-257.33	-	exergonic
Mo-R058	4Mo + N2 = 2Mo2N	7.30	-163.18	686.8	exergonic
Ni-R104	6Ni + N2 = 2Ni3N	7.95	1.67	-	endergonic
Sr-R103	4Sr + N2 = 2Sr2N	7.99	-388.99	-	exergonic
W-R37	4W + N2 = 2W2N	3.81	-283.98	-	exergonic
Zn-R54	3Zn + N2 = Zn3N2	14.28	-22.17	-	endergonic

Table S28: Hydrogenation reactions examined in the Ellingham diagram of Figure 2b.

ID	Reaction	dm_stoich [%]	h298 [kJ/mol]	T_eq [°C]	Type
Al-R15	2/3AlN + H2 = 2/3Al + 2/3NH3	-34.17	181.39	-	endergonic
Ca-R040	2/3Ca2N + H2 = 4/3Ca + 2/3NH3	-14.88	142.63	-	endergonic
Co-R022	2/3Co3N + H2 = 2Co + 2/3NH3	-7.34	-36.18	-	exergonic
Cr-R009	2/3Cr2N + H2 = 4/3Cr + 2/3NH3	-11.87	53.08	-	endergonic
Cu-R21	2/9CuN3 + H2 = 2/9Cu + 2/3NH3	-39.81	-55.8	-	exergonic
Fe-R054	2/3Fe3N + H2 = 2Fe + 2/3NH3	-7.72	9.99	415.8	exergonic
Li-R033	2/3Li3N + H2 = 2Li + 2/3NH3	-40.22	79.11	-	endergonic
Mn-R36	2/3Mn4N + H2 = 8/3Mn + 2/3NH3	-5.99	55.18	-	endergonic
Mo-R016	2/3Mo2N + H2 = 4/3Mo + 2/3NH3	-6.80	23.79	-	endergonic
Ni-R035	2/3Ni3N + H2 = 2Ni + 2/3NH3	-7.37	-31.16	-	exergonic
Sr-R020	2/3Sr2N + H2 = 4/3Sr + 2/3NH3	-7.40	99.07	-	endergonic
W-R01	2/3W2N + H2 = 4/3W + 2/3NH3	-3.67	64.06	-	endergonic
Zn-R31	1/3Zn3N2 + H2 = Zn + 2/3NH3	-12.50	-23.21	-	exergonic

1.6 Ellingham diagrams

Ellingham diagrams of all identified reactions (see Section 1.4 Reactions): standard Gibbs free energy change per mol of N_2 (nitridation) and per mole of H_2 (hydrogenation) as a function of temperature. Dashed lines indicate species from the MP database with an E_{hull} greater than 0, i.e. potentially unstable at standard conditions.

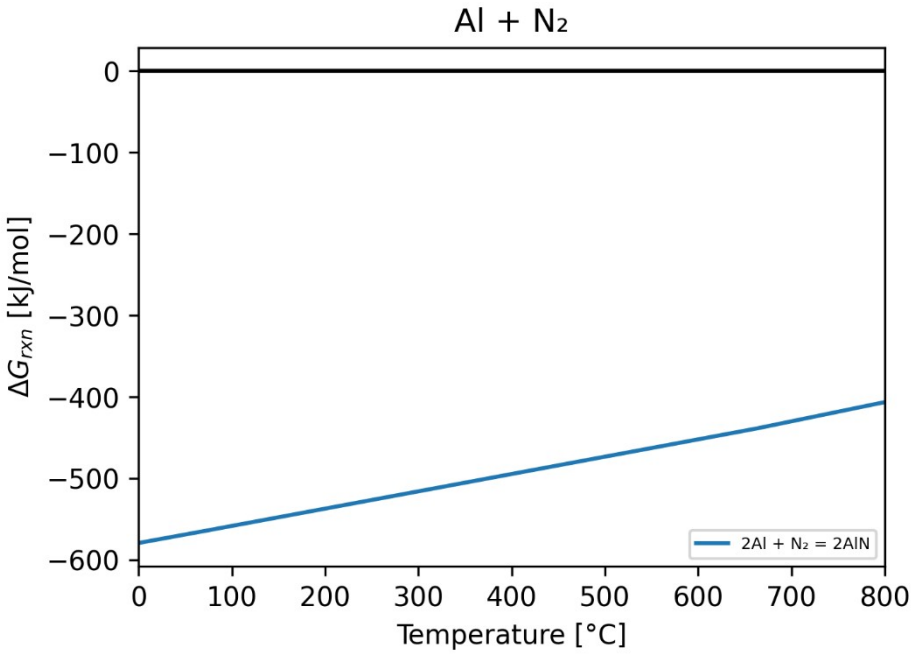

Figure S2: Ellingham diagram of the Al nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

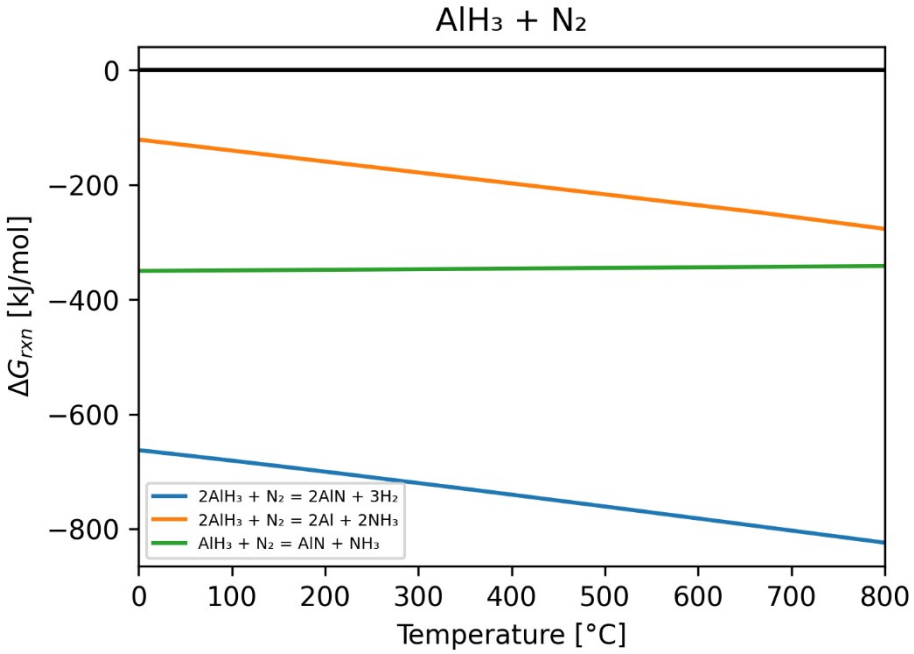

Figure S3: Ellingham diagram of the AlH_3 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

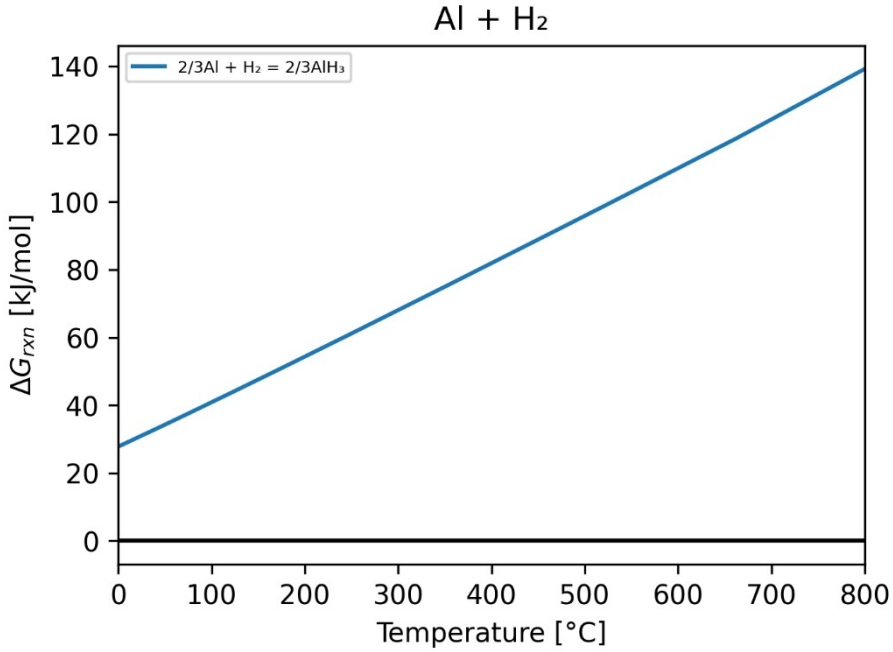

Figure S4: Ellingham diagram of the Al hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

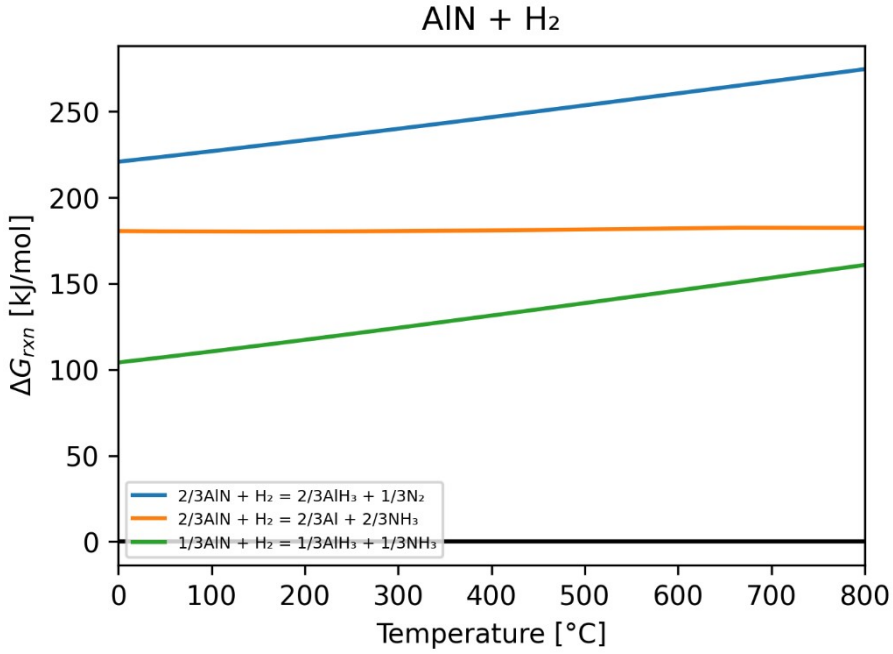

Figure S5: Ellingham diagram of the AlN hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

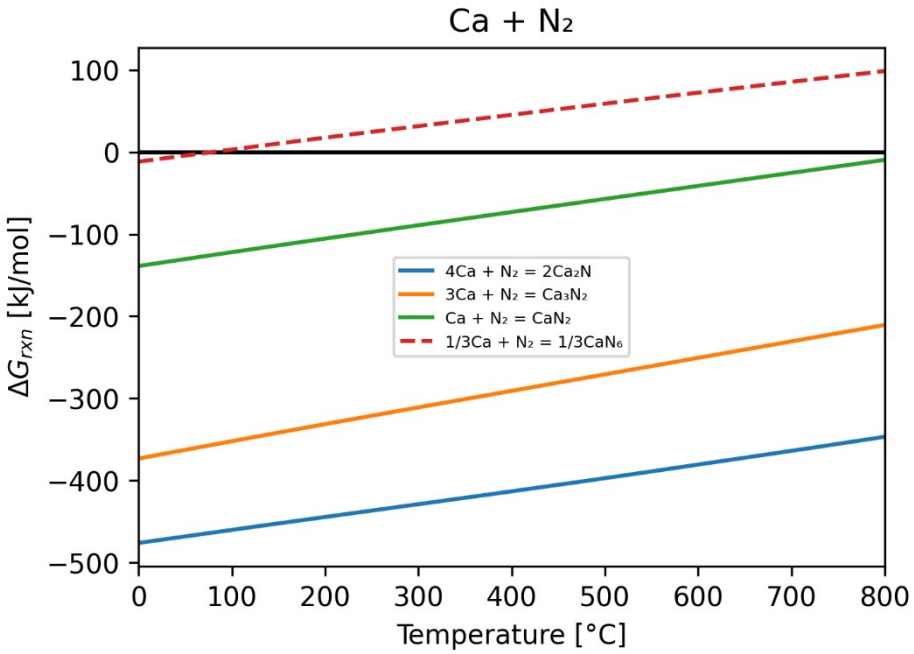

Figure S6: Ellingham diagram of the Ca nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

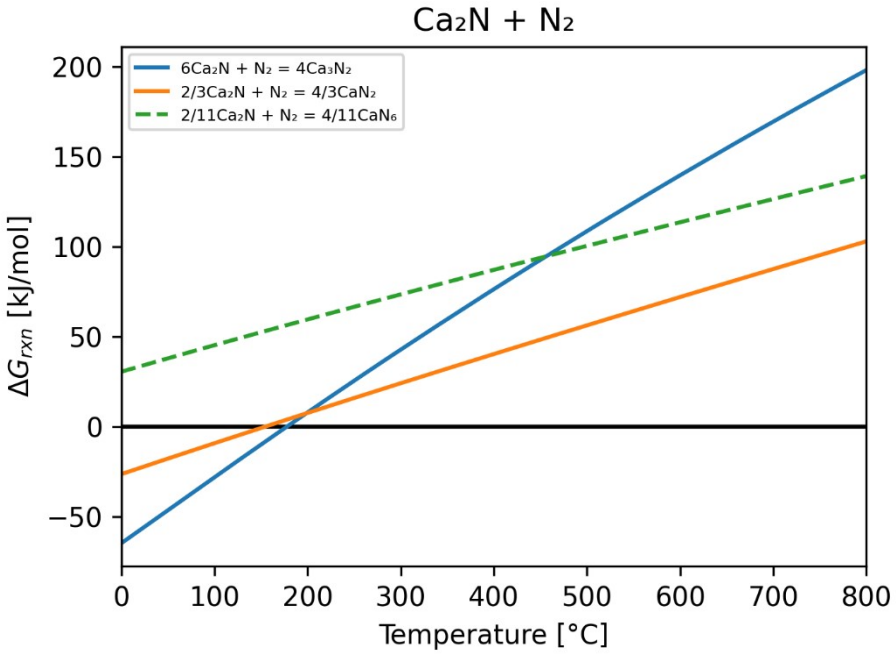

Figure S7: Ellingham diagram of the Ca_2N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

Figure S8: Ellingham diagram of the Ca_2N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

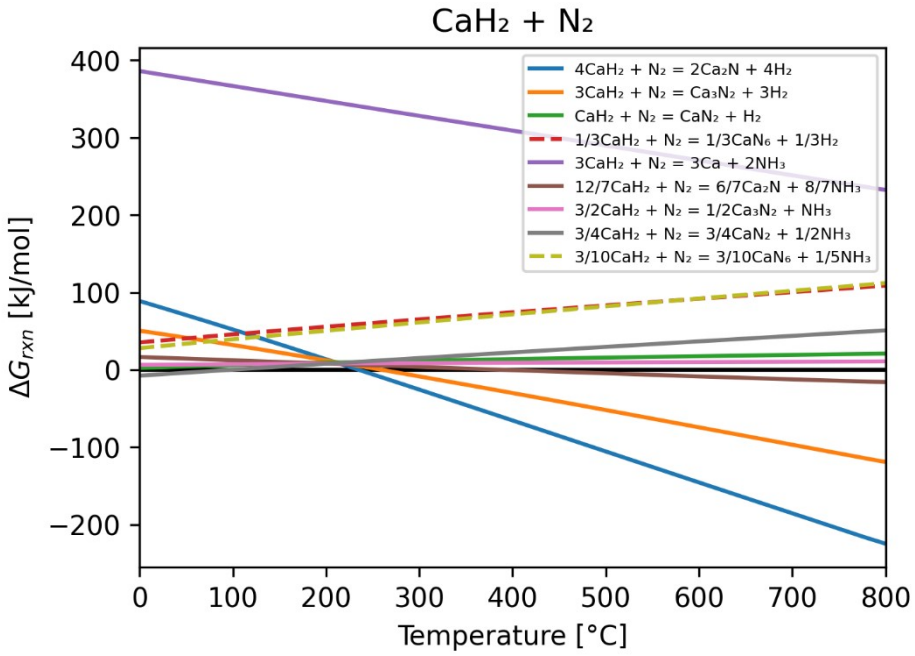

Figure S9: Ellingham diagram of the CaH_2 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

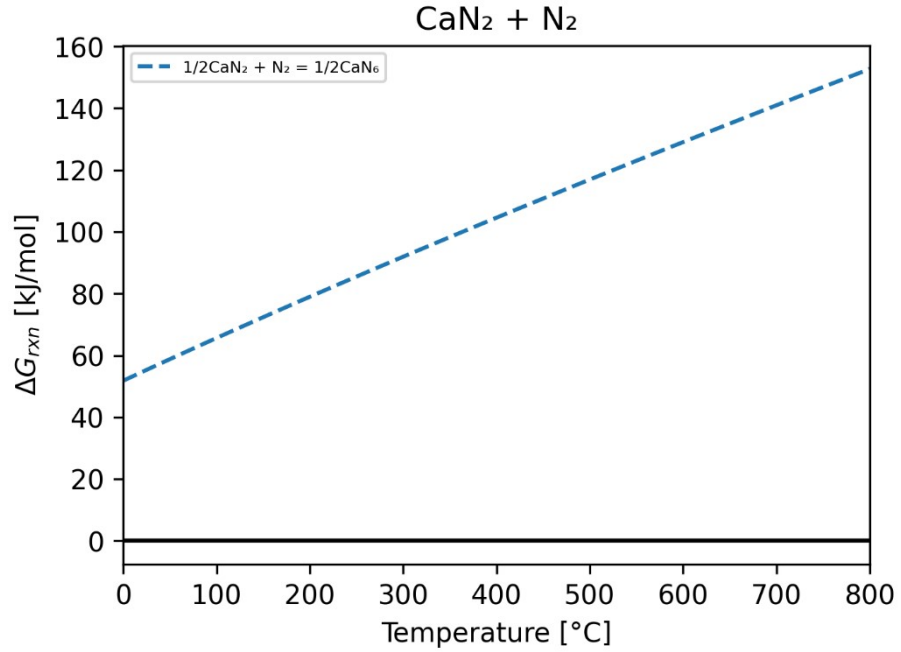

Figure S10: Ellingham diagram of the CaN_2 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

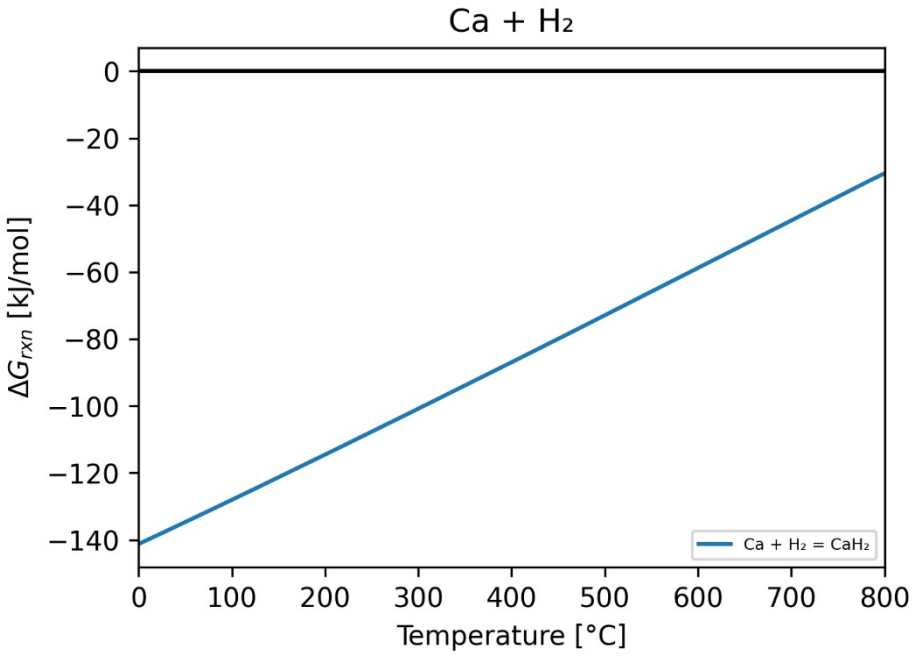

Figure S11: Ellingham diagram of the Ca hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

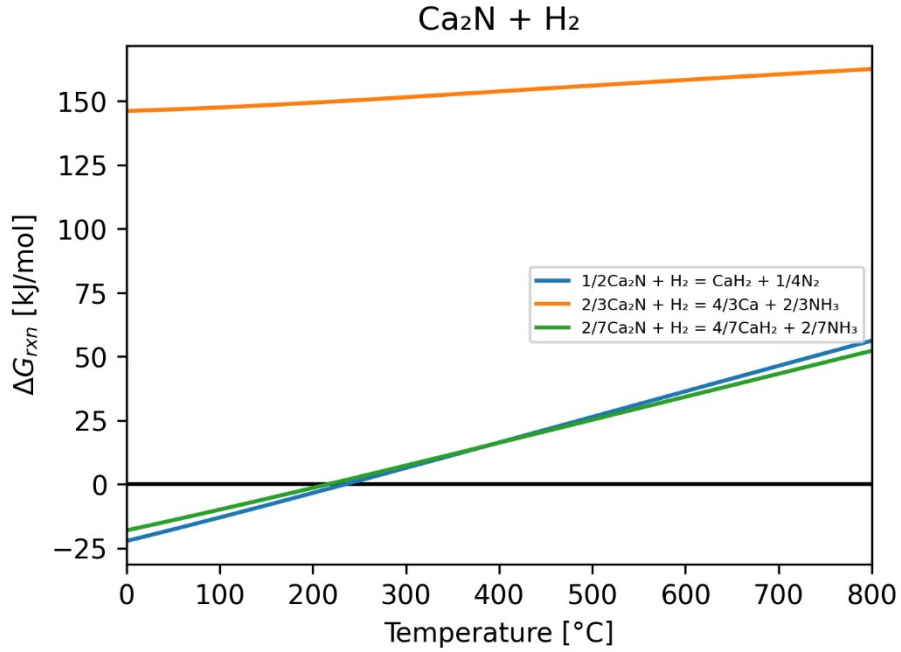

Figure S12: Ellingham diagram of the Ca_2N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

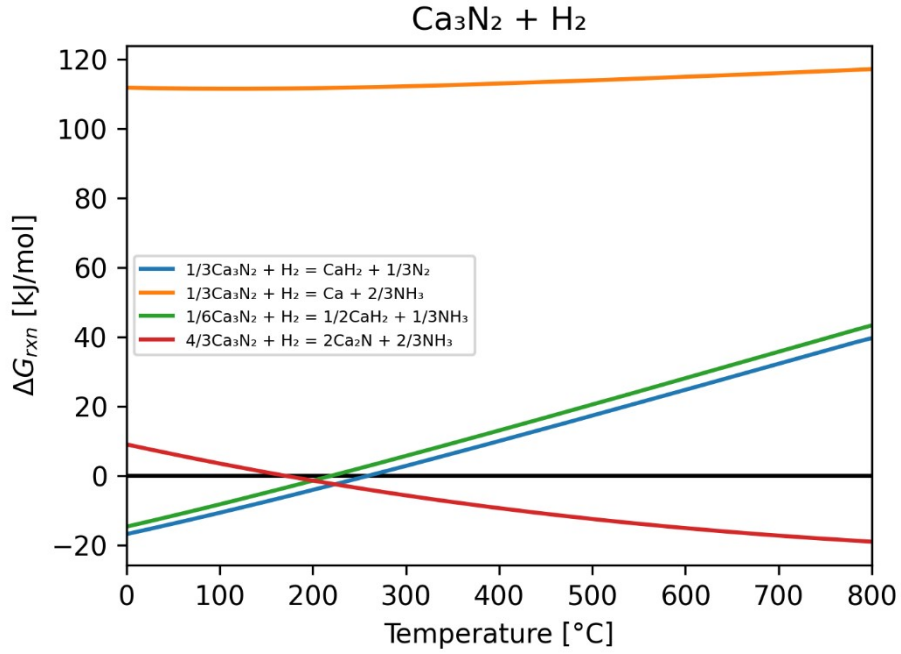

Figure S13: Ellingham diagram of the Ca_3N_2 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

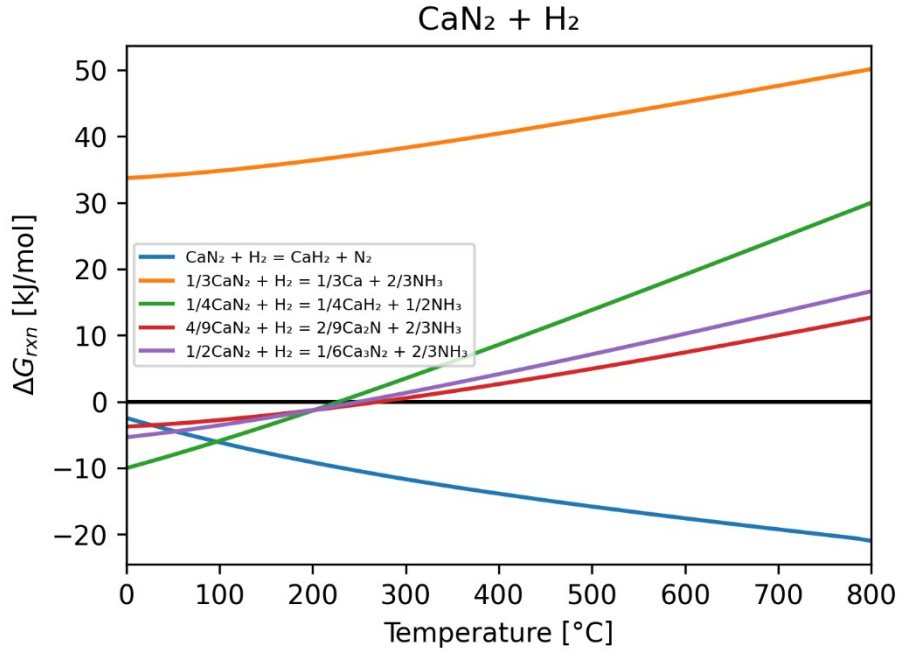

Figure S14: Ellingham diagram of the CaN_2 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

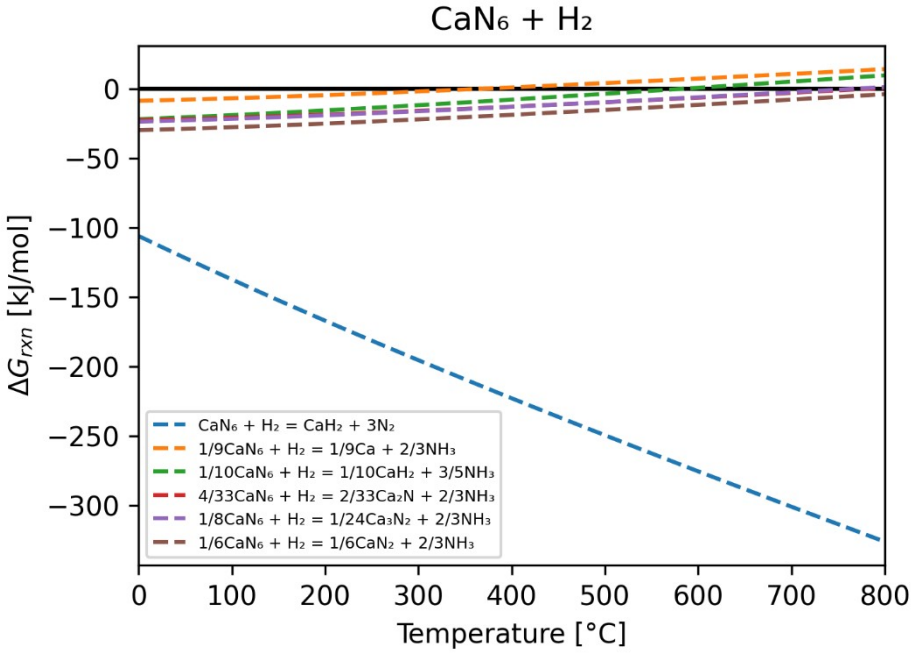

Figure S15: Ellingham diagram of the CaN_6 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

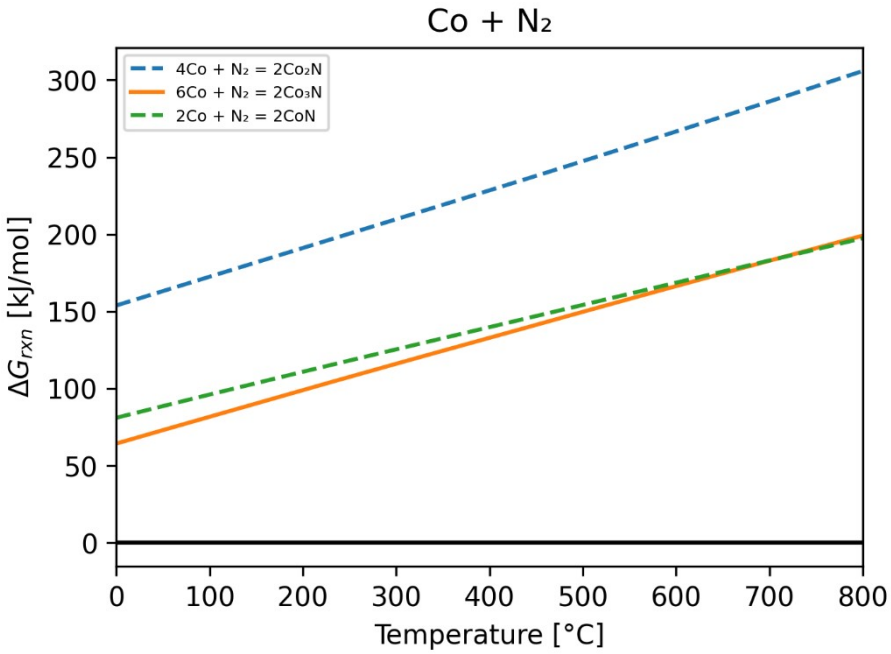

Figure S16: Ellingham diagram of the Co nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

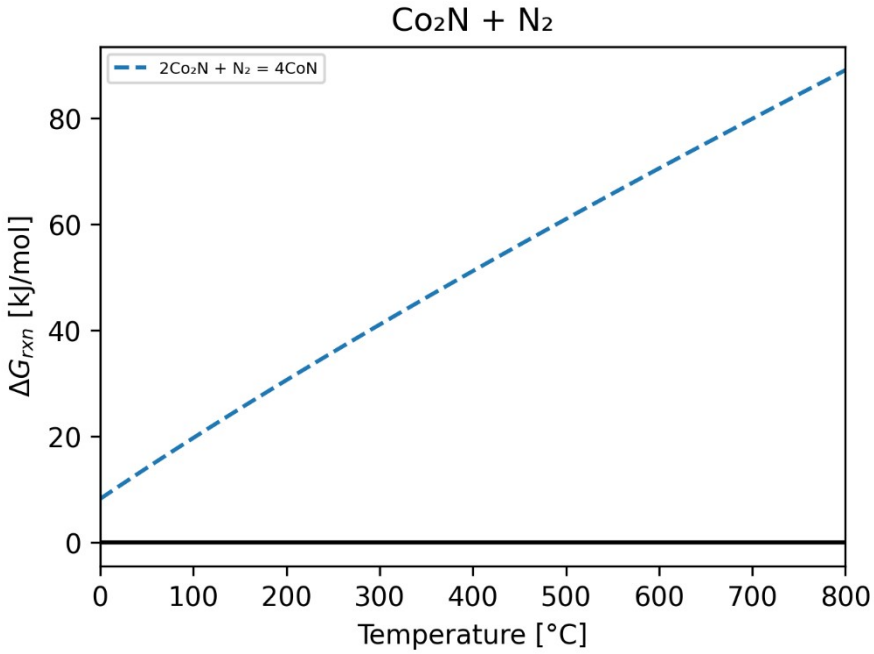

Figure S17: Ellingham diagram of the Co_2N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

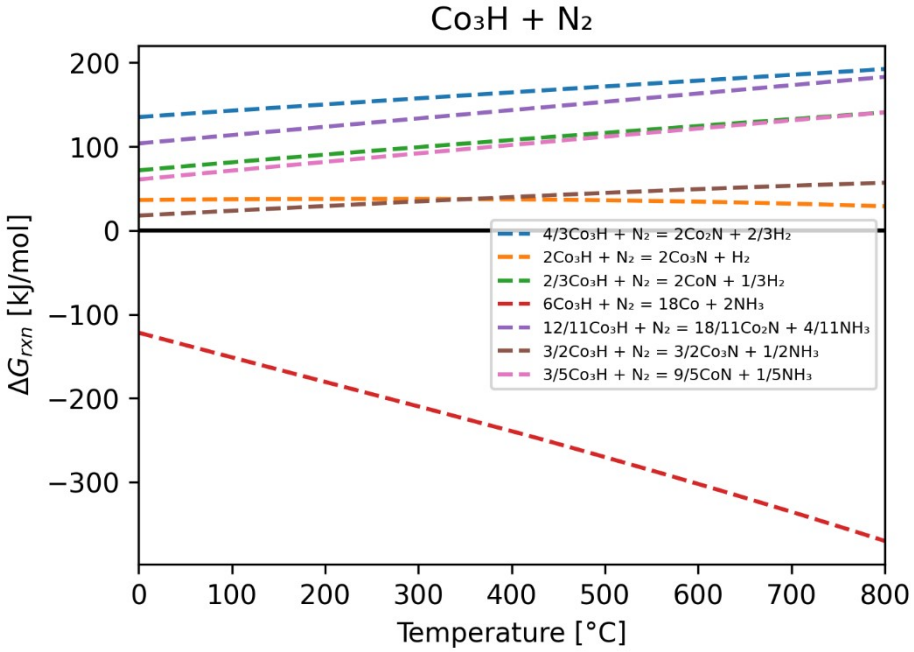

Figure S18: Ellingham diagram of the Co_3H nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

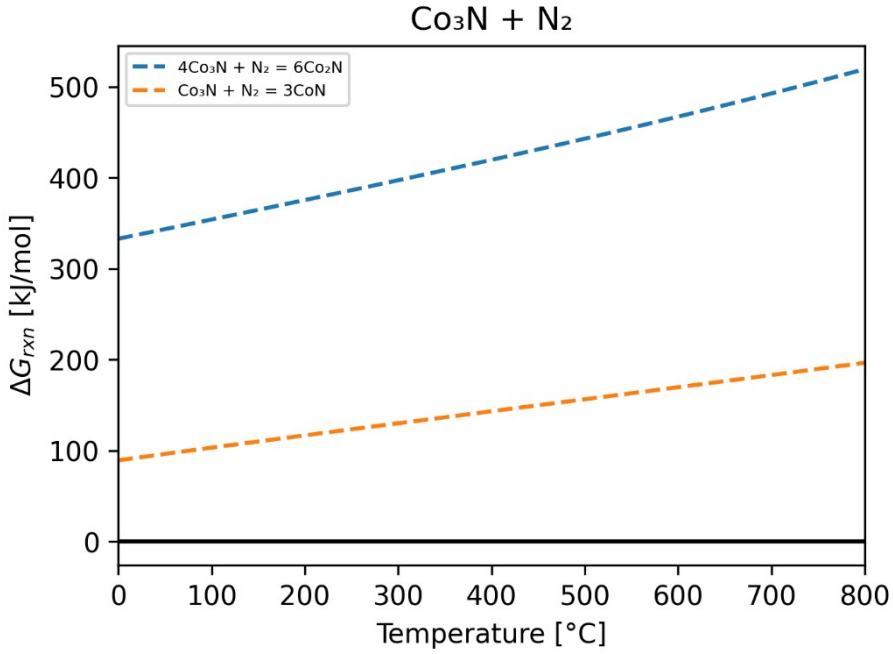

Figure S19: Ellingham diagram of the Co_3N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

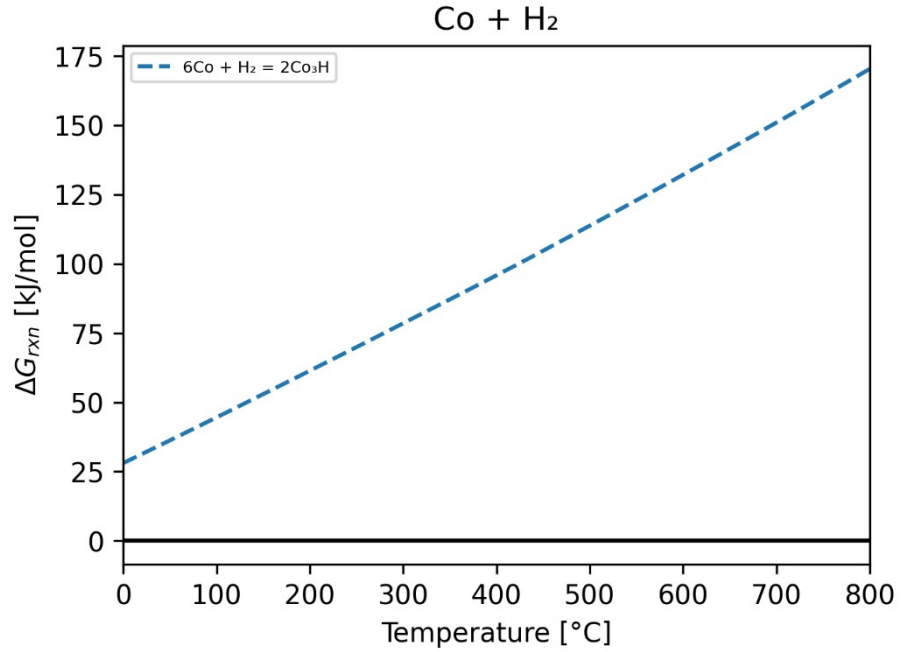

Figure S20: Ellingham diagram of the Co hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

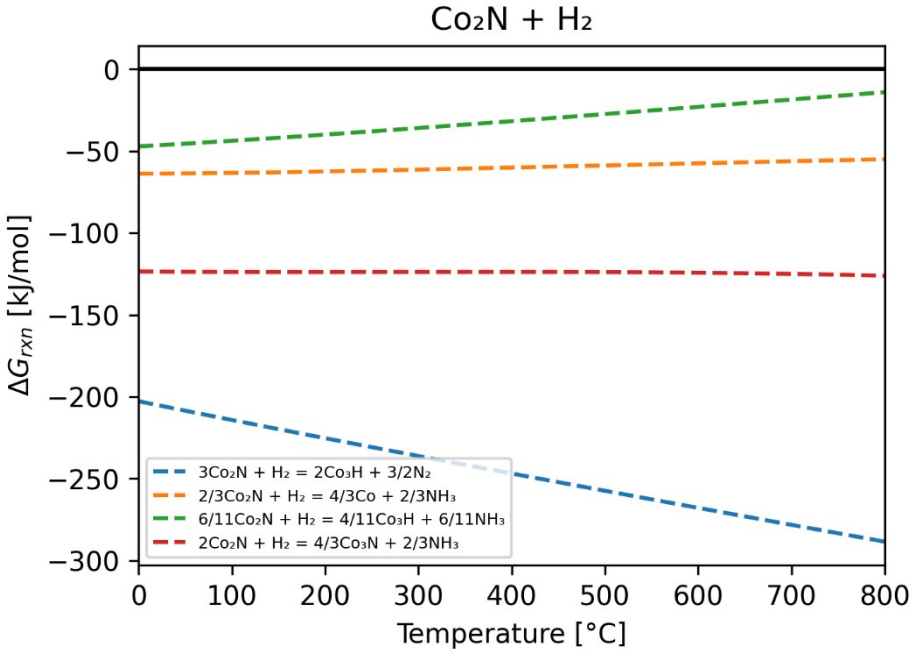

Figure S21: Ellingham diagram of the Co_2N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

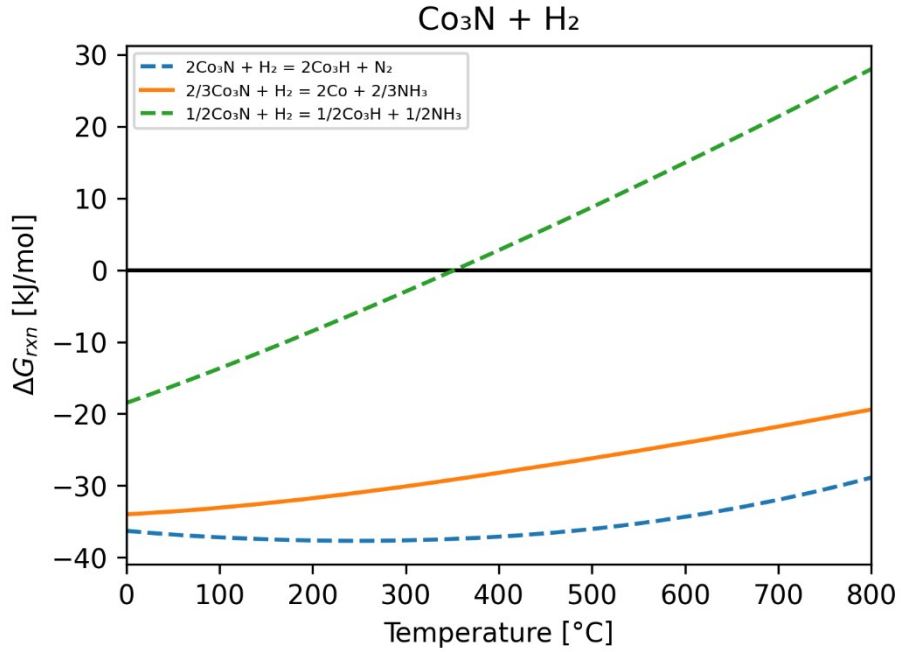

Figure S22: Ellingham diagram of the Co_3N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

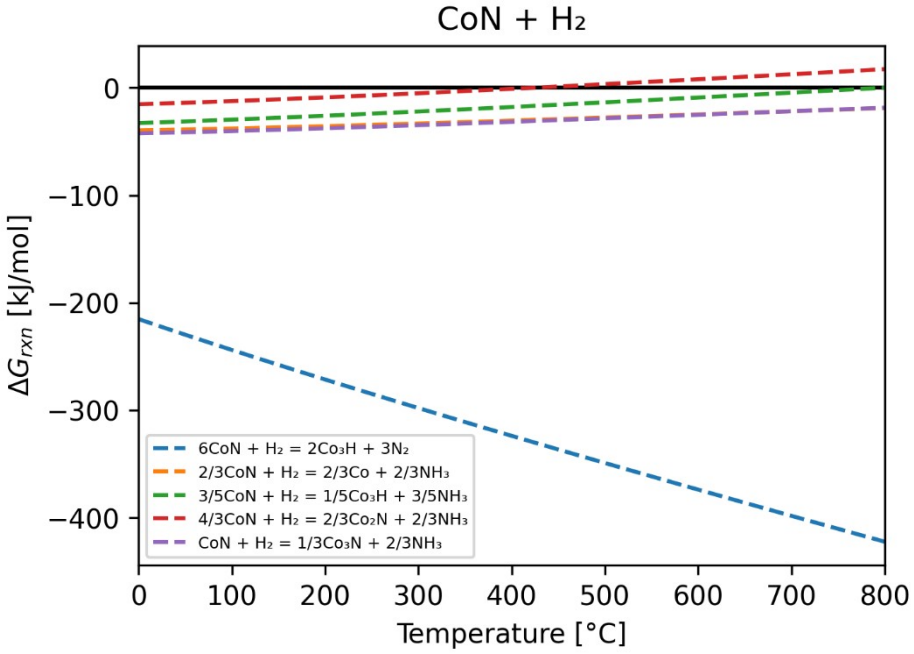

Figure S23: Ellingham diagram of the CoN hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

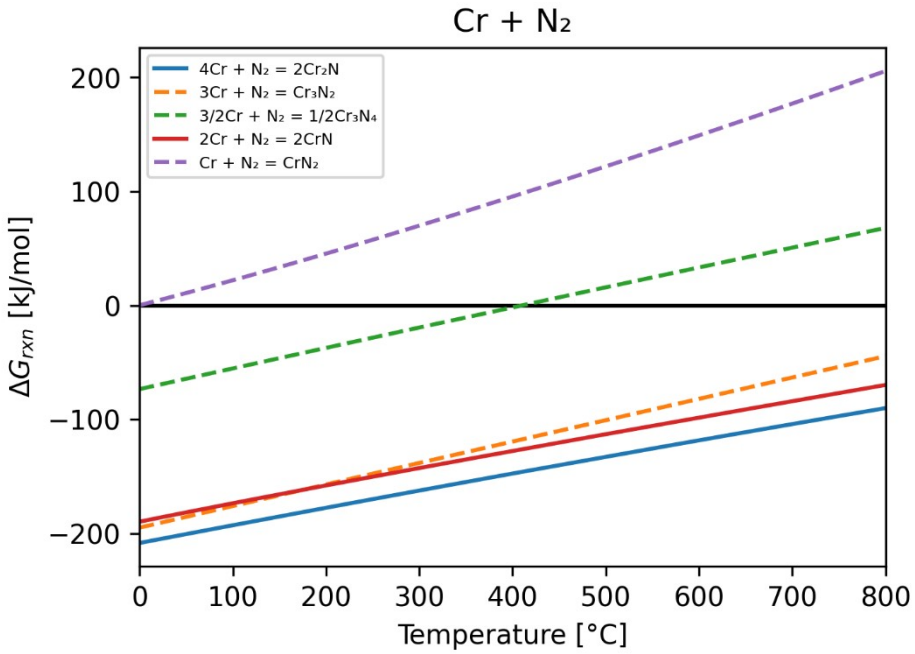

Figure S24: Ellingham diagram of the Cr nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

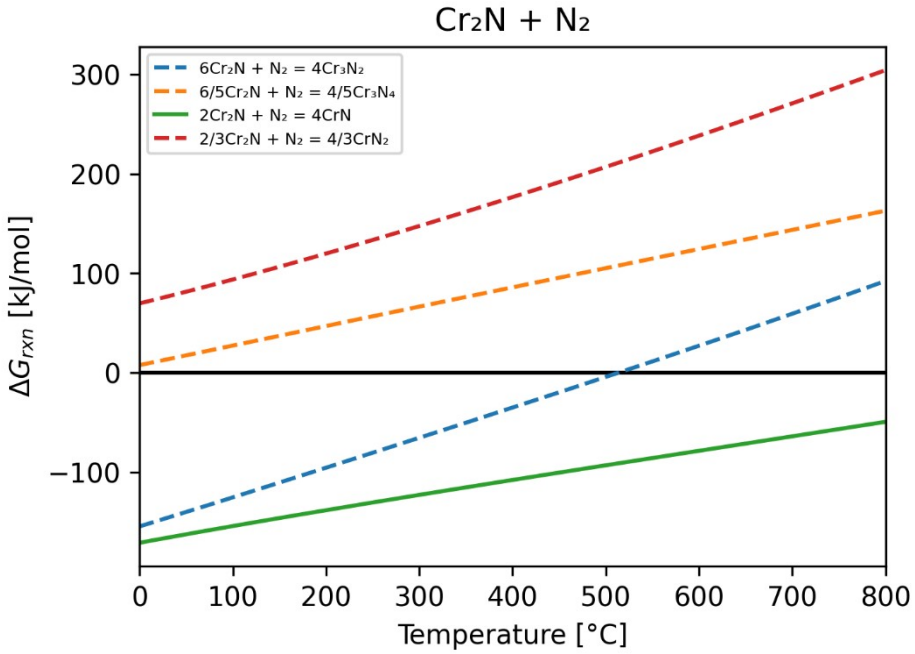

Figure S25: Ellingham diagram of the Cr_2N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

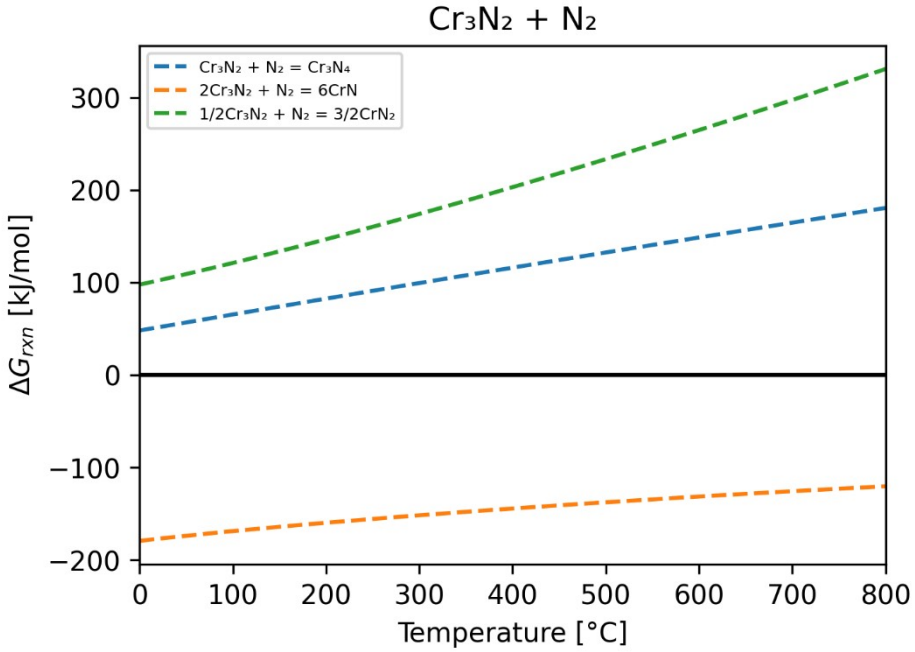

Figure S26: Ellingham diagram of the Cr_3N_2 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

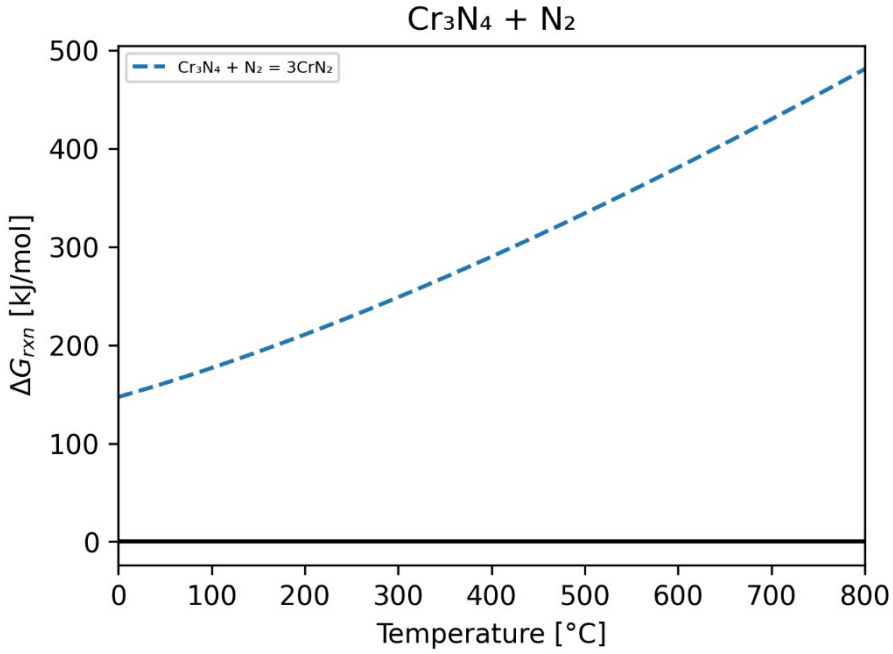

Figure S27: Ellingham diagram of the Cr_3N_4 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

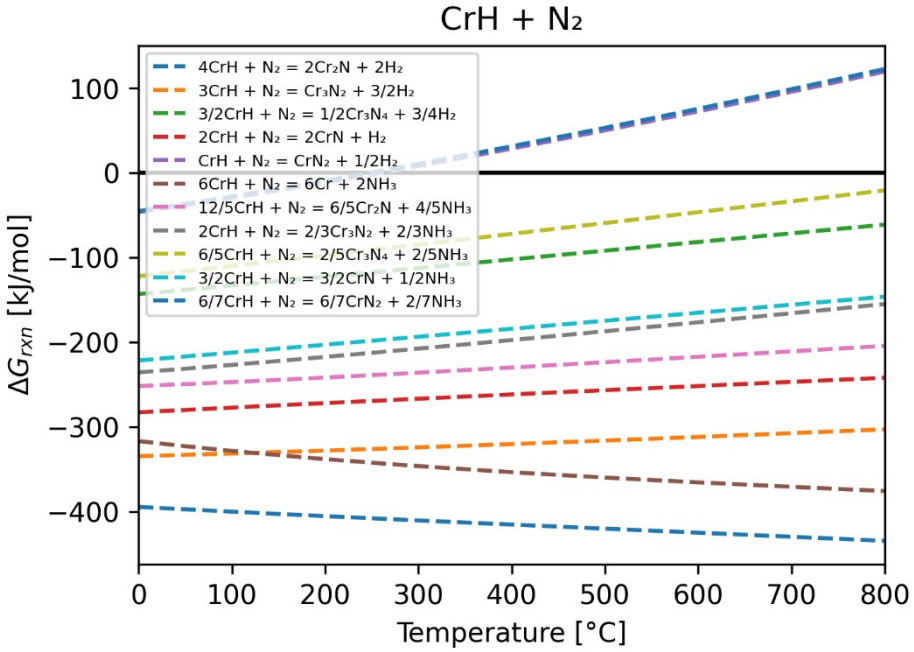

Figure S28: Ellingham diagram of the CrH nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

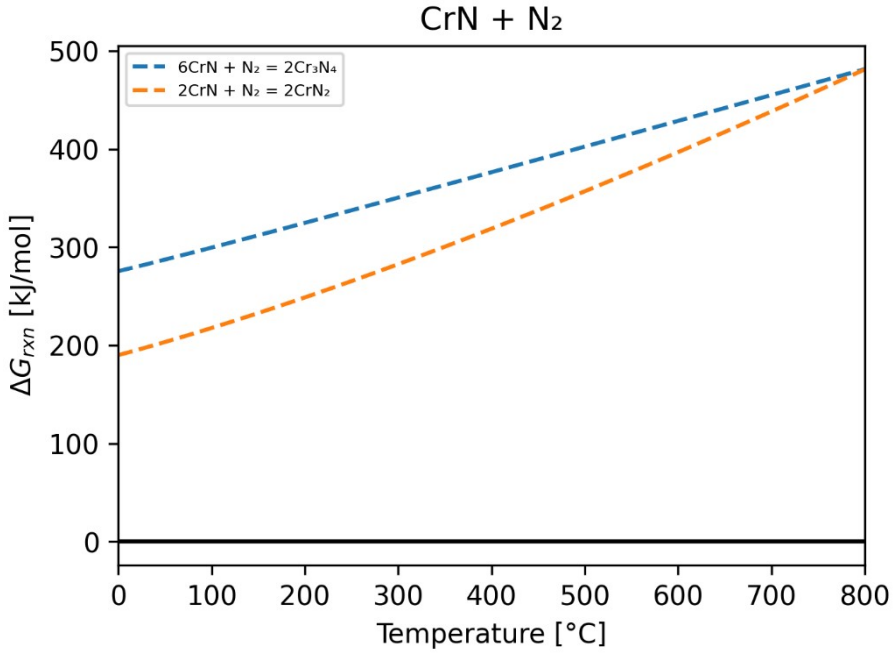

Figure S29: Ellingham diagram of the CrN nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

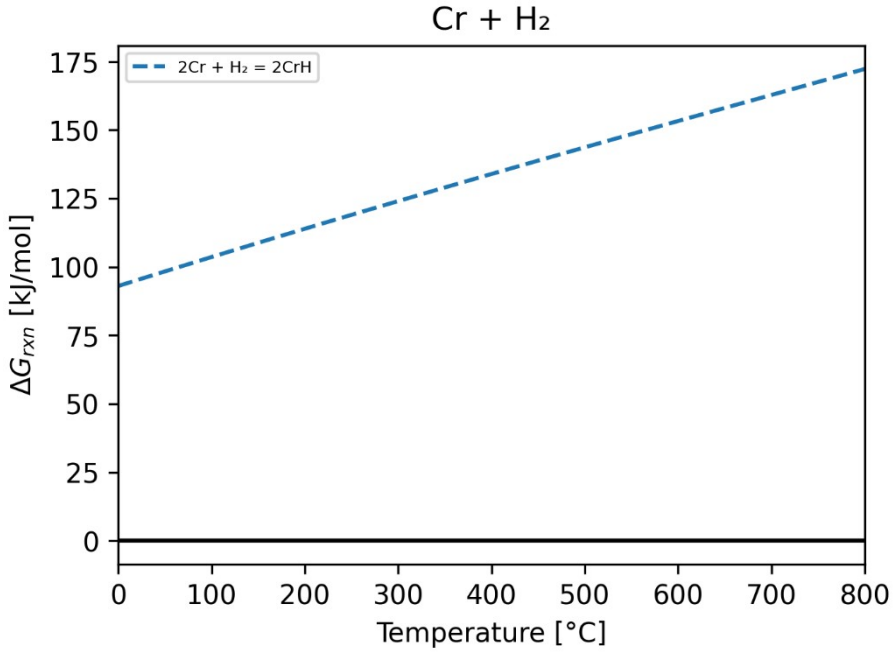

Figure S30: Ellingham diagram of the Cr hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

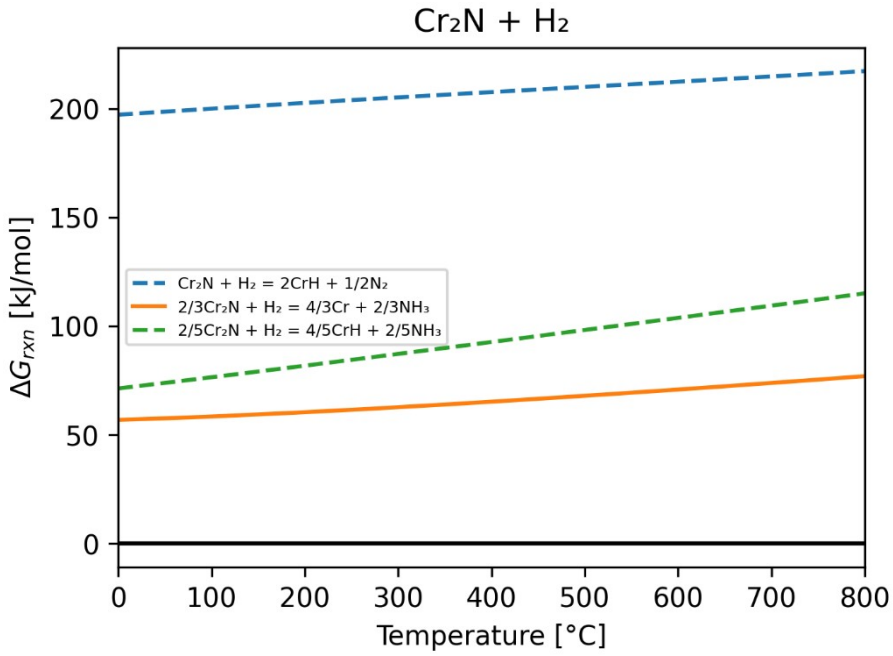

Figure S31: Ellingham diagram of the Cr_2N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

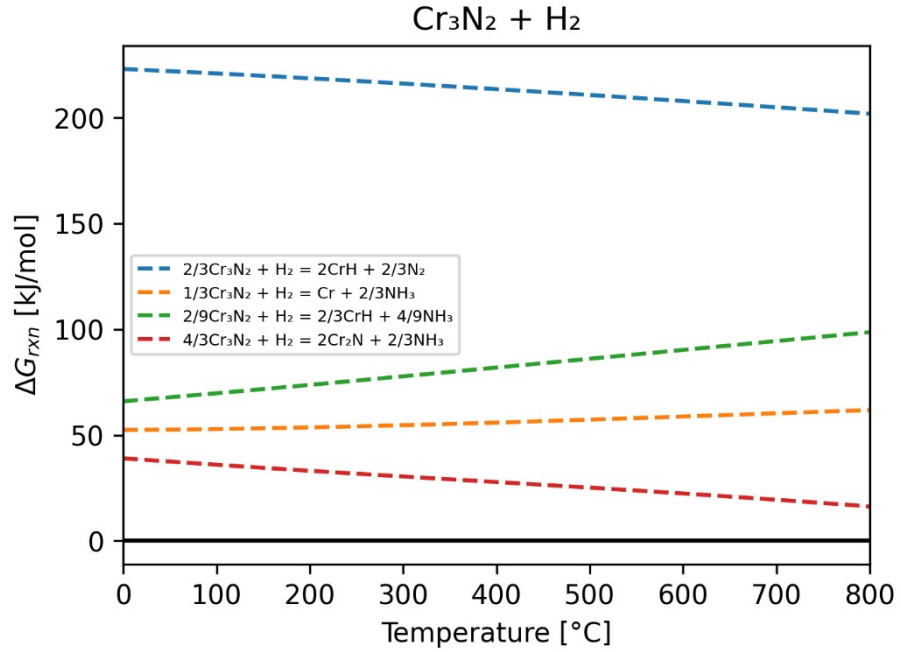

Figure S32: Ellingham diagram of the Cr_3N_2 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

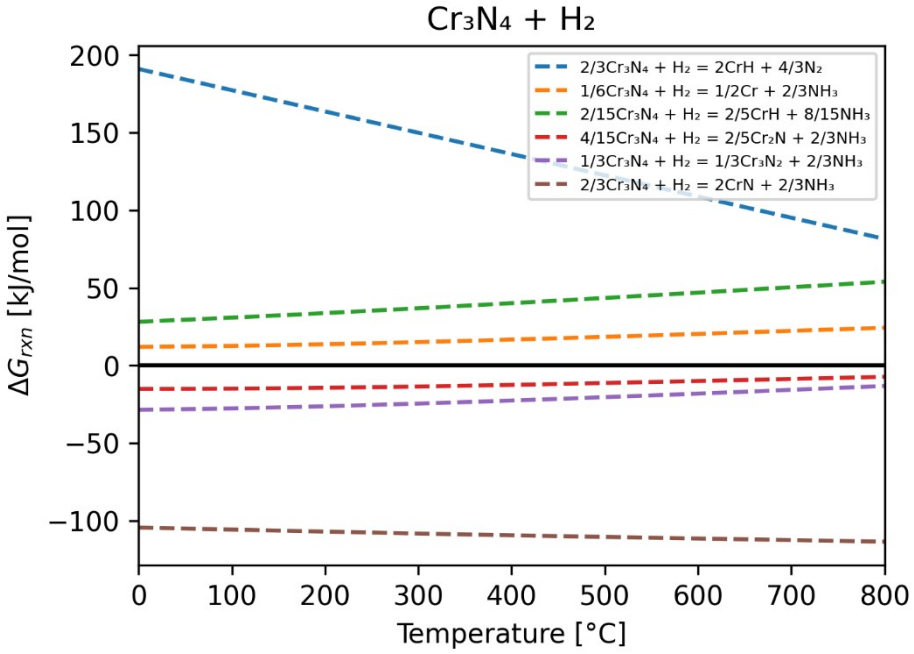

Figure S33: Ellingham diagram of the Cr_3N_4 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

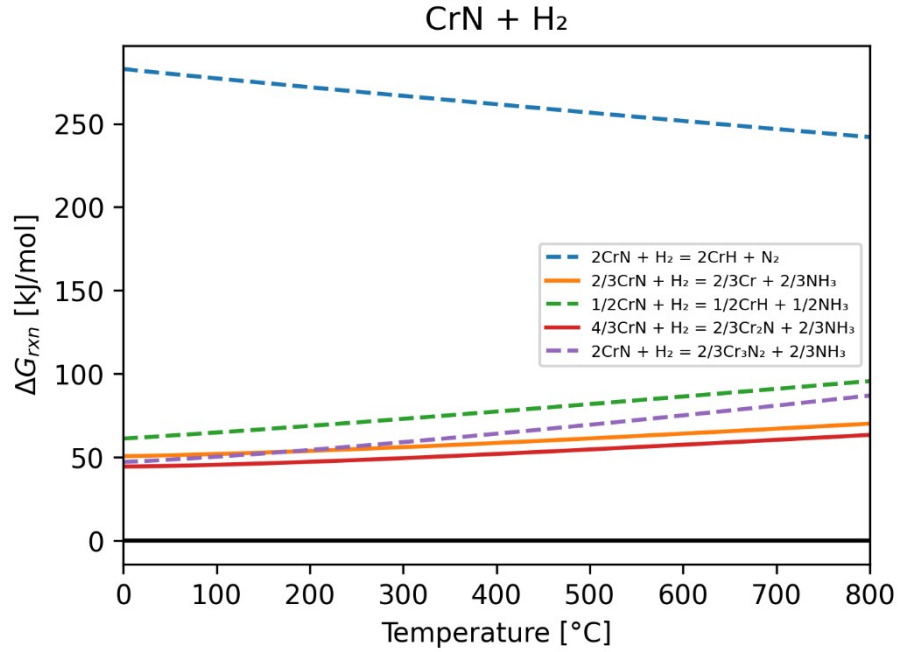

Figure S34: Ellingham diagram of the CrN hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

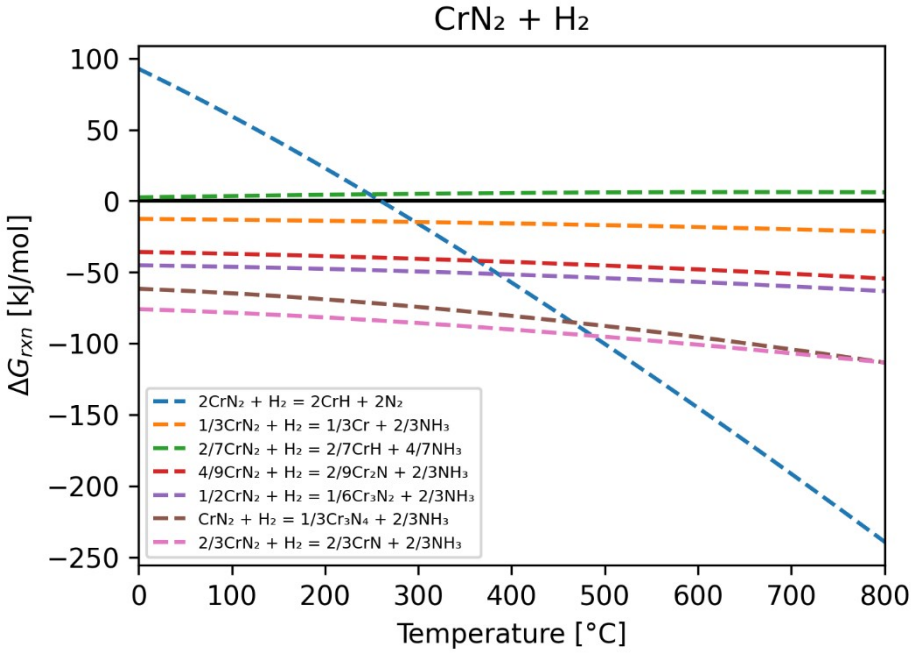

Figure S35: Ellingham diagram of the CrN_2 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

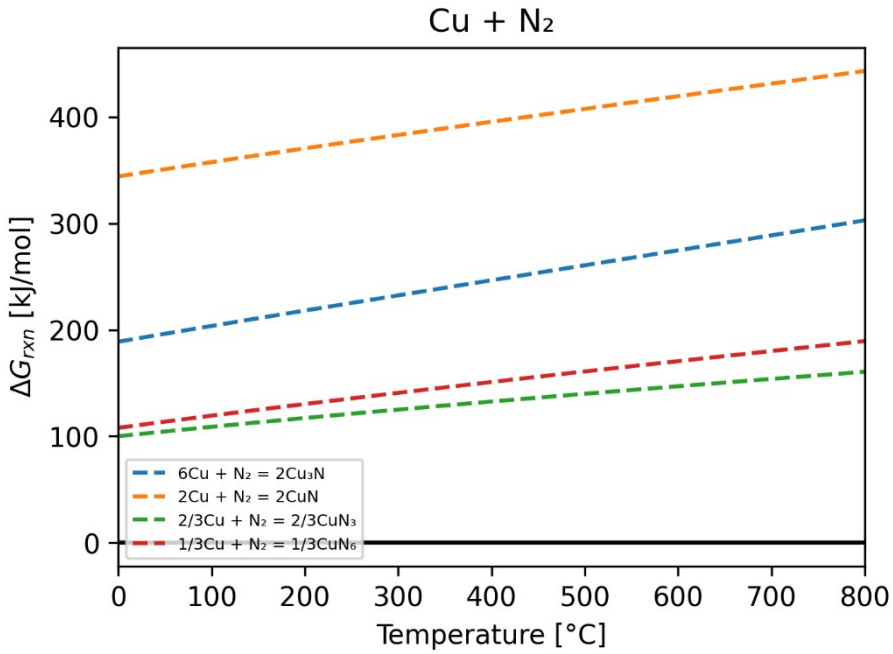

Figure S36: Ellingham diagram of the Cu nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

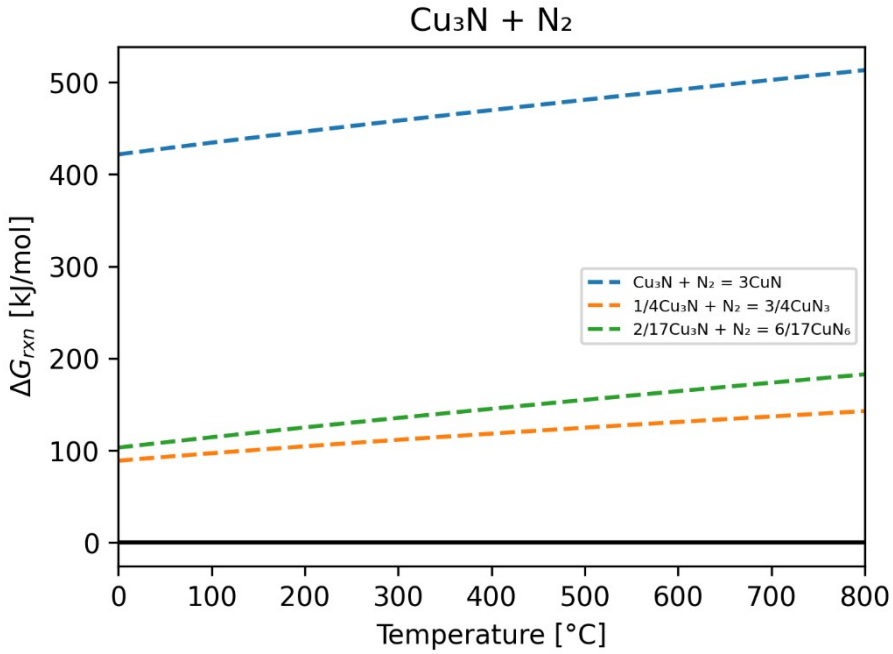

Figure S37: Ellingham diagram of the Cu_3N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

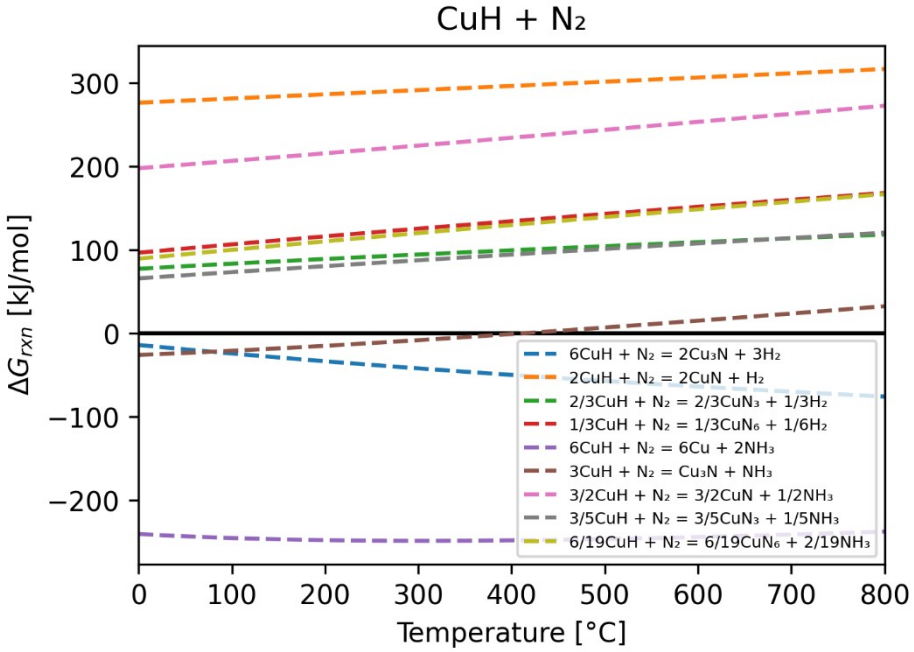

Figure S38: Ellingham diagram of the CuH nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

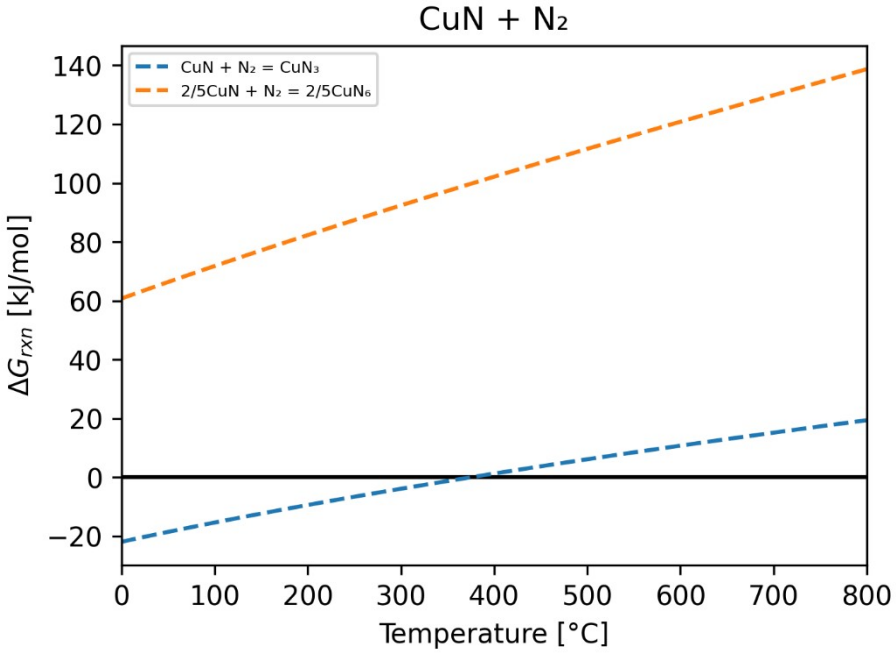

Figure S39: Ellingham diagram of the CuN nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

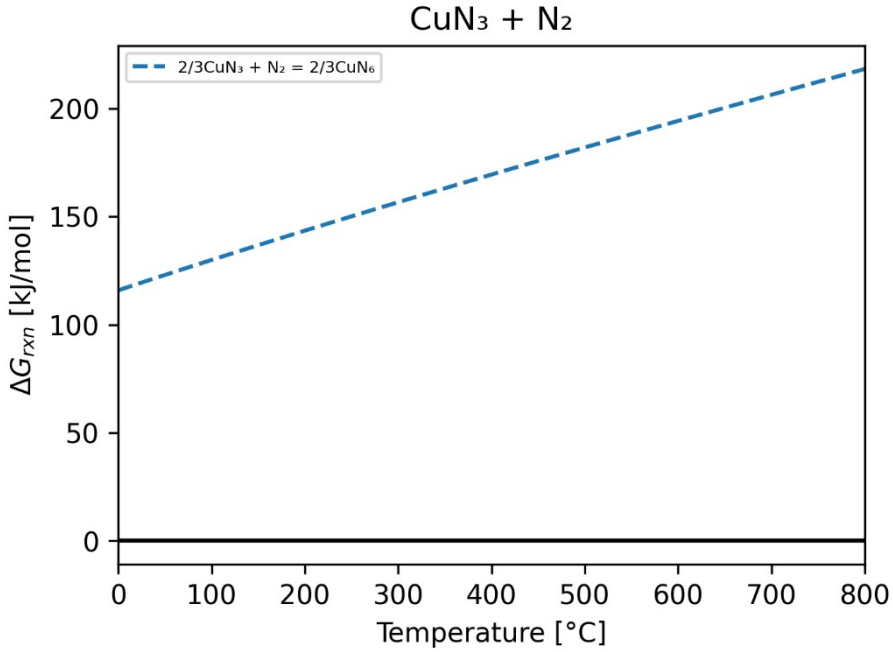

Figure S40: Ellingham diagram of the CuN_3 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

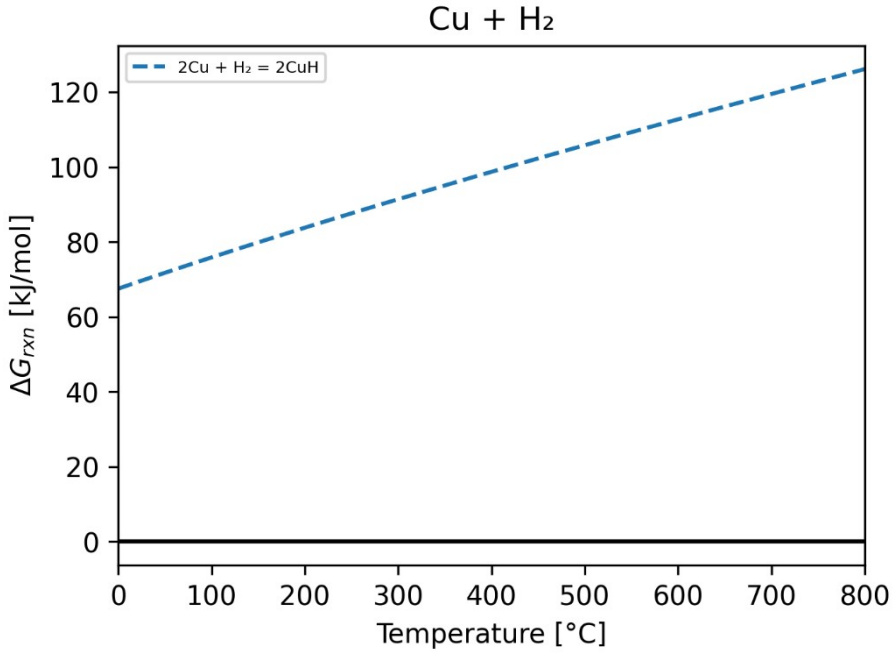

Figure S41: Ellingham diagram of the Cu hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

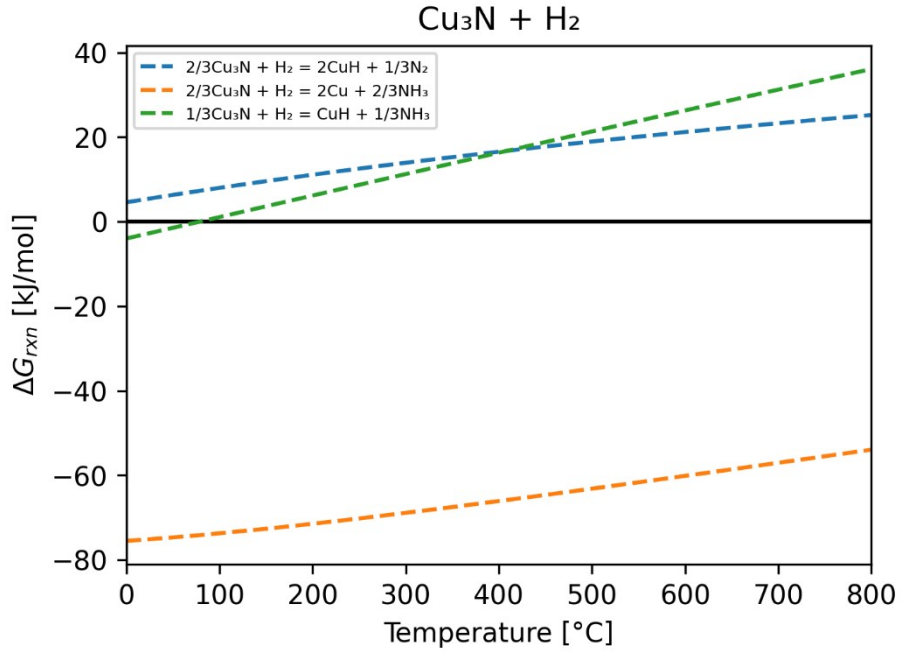

Figure S42: Ellingham diagram of the Cu_3N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

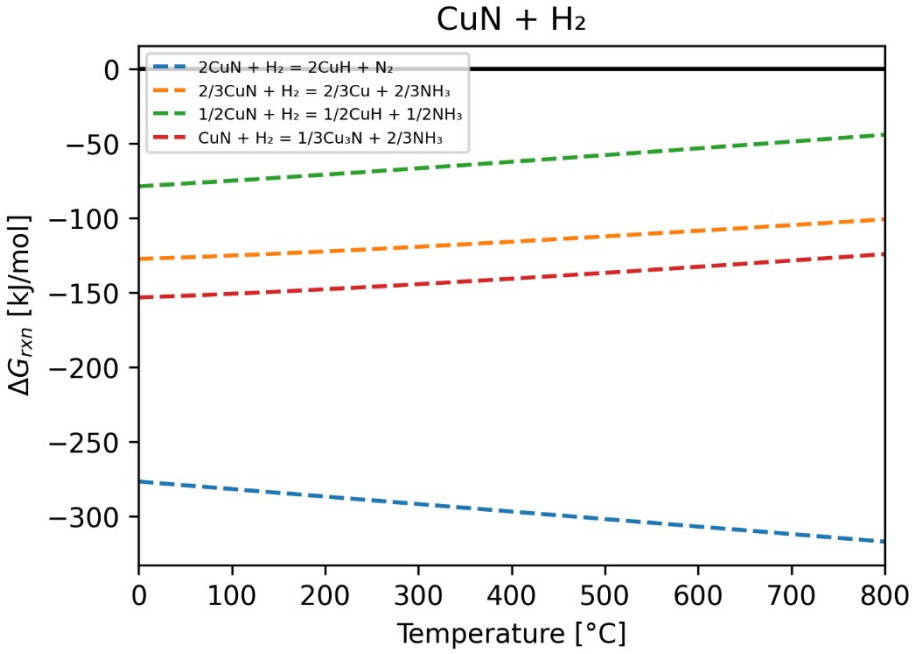

Figure S43: Ellingham diagram of the CuN hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

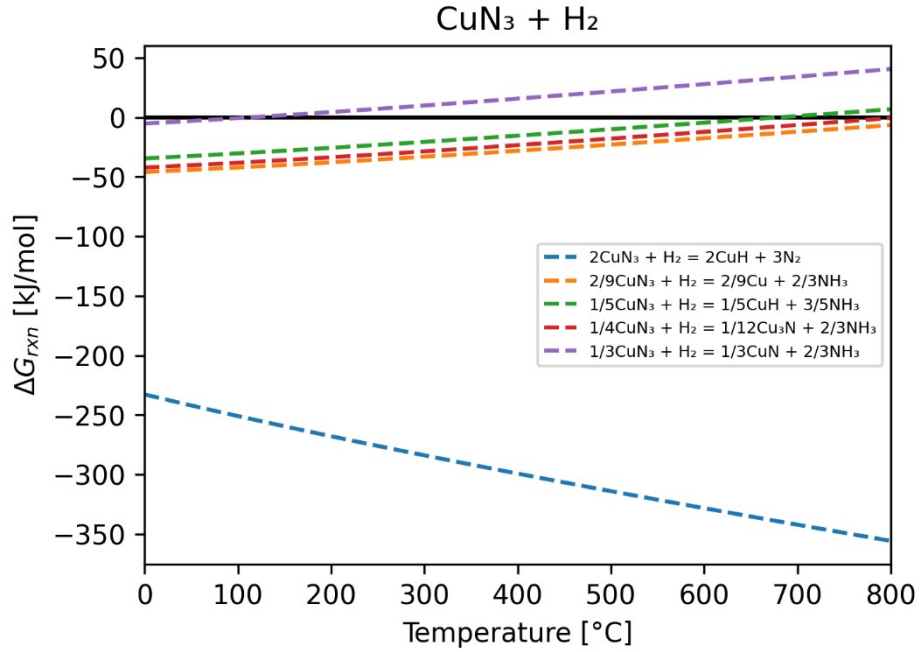

Figure S44: Ellingham diagram of the CuN_3 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

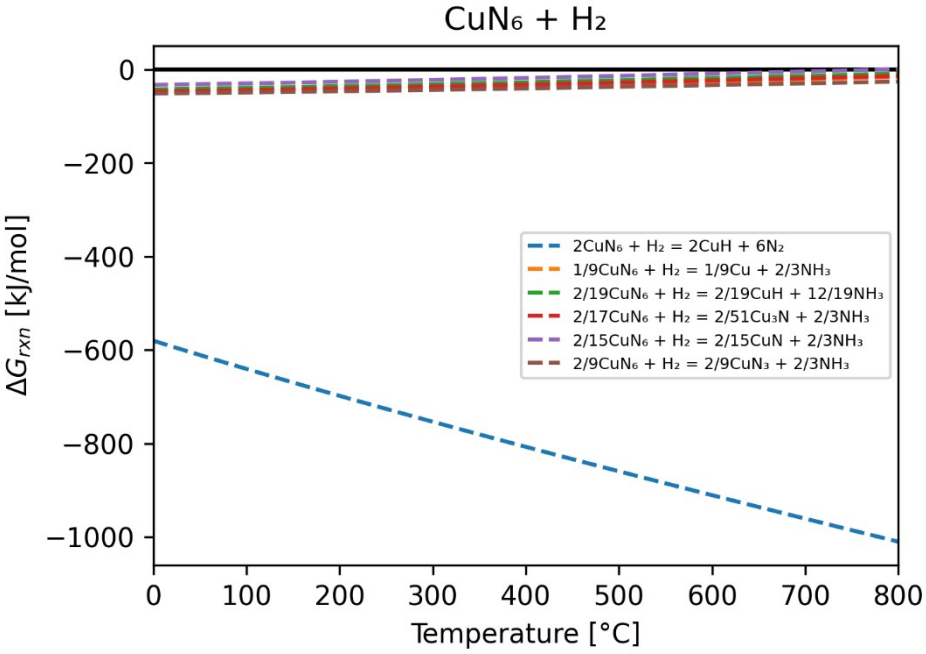

Figure S45: Ellingham diagram of the CuN_6 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

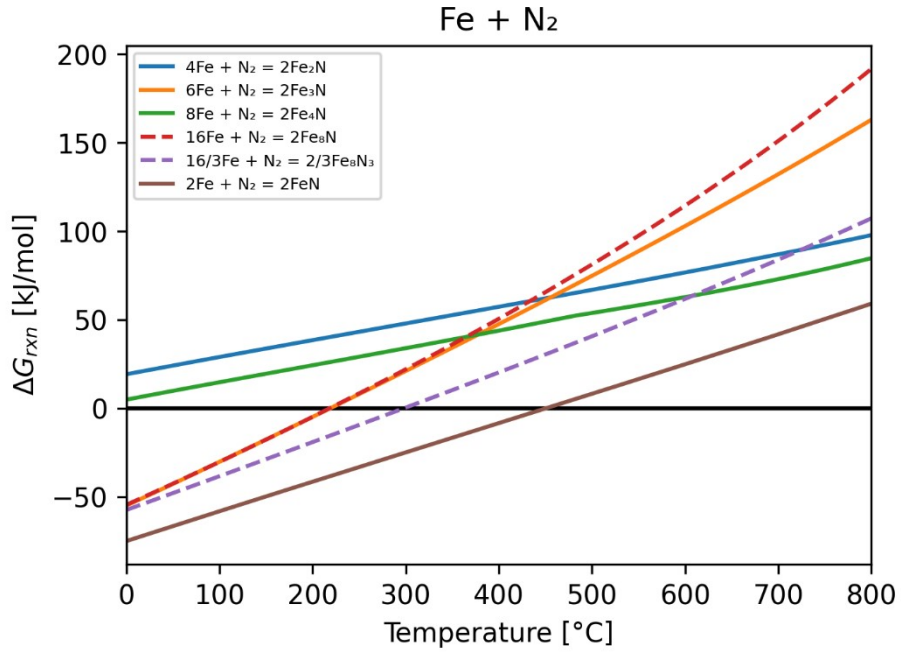

Figure S46: Ellingham diagram of the Fe nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

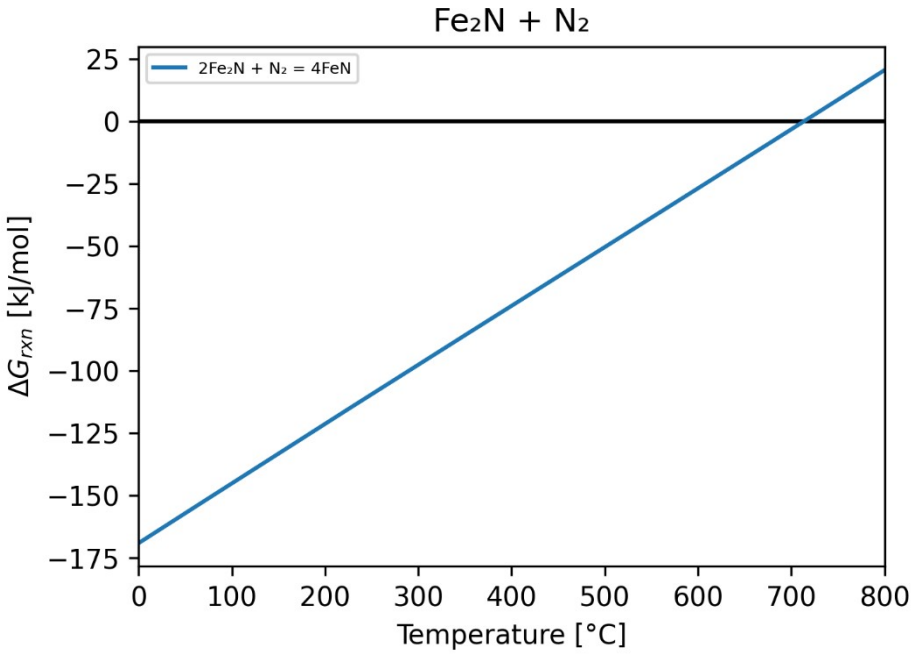

Figure S47: Ellingham diagram of the Fe_2N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

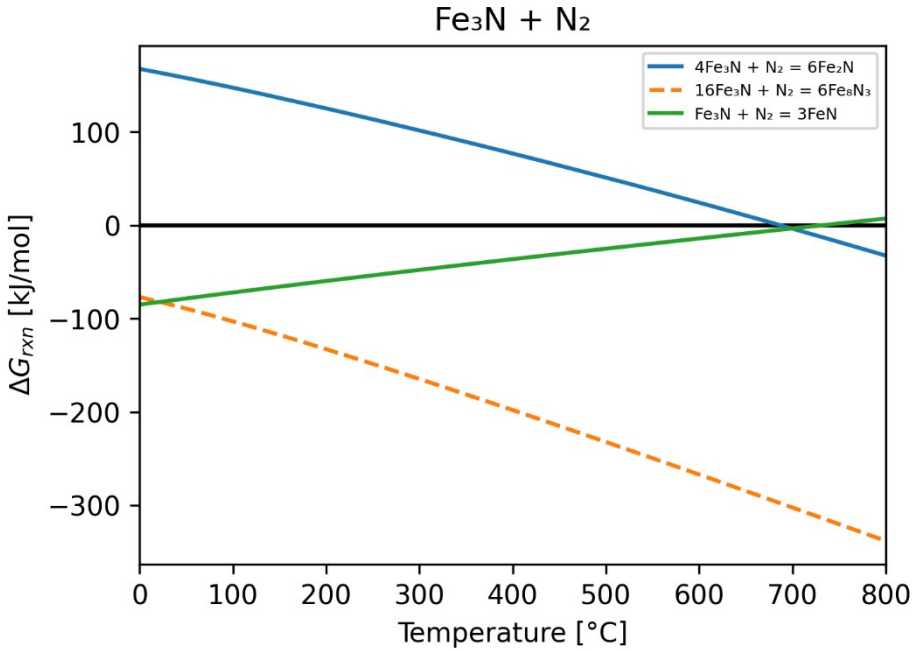

Figure S48: Ellingham diagram of the Fe_3N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

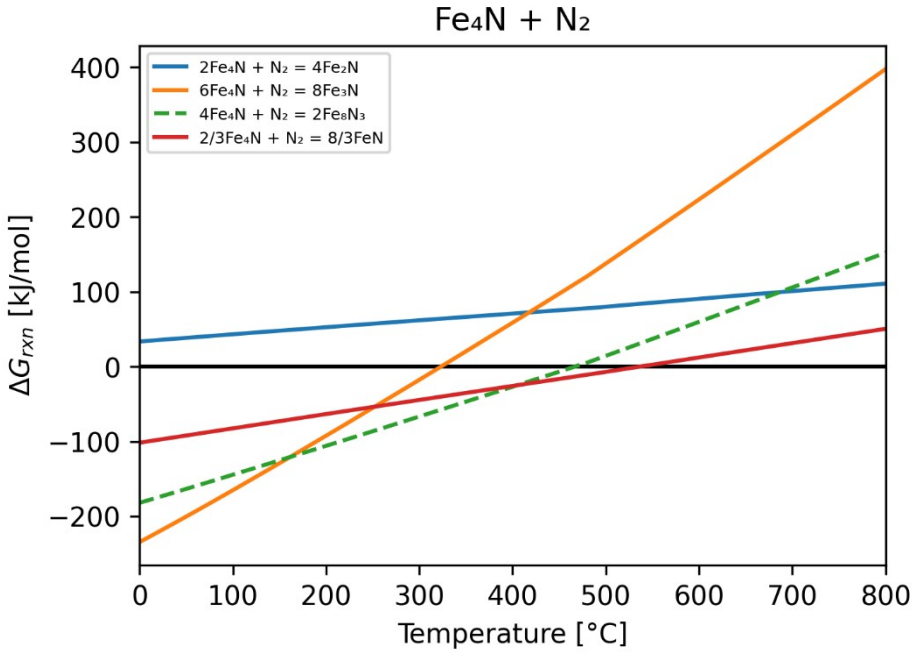

Figure S49: Ellingham diagram of the Fe_4N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

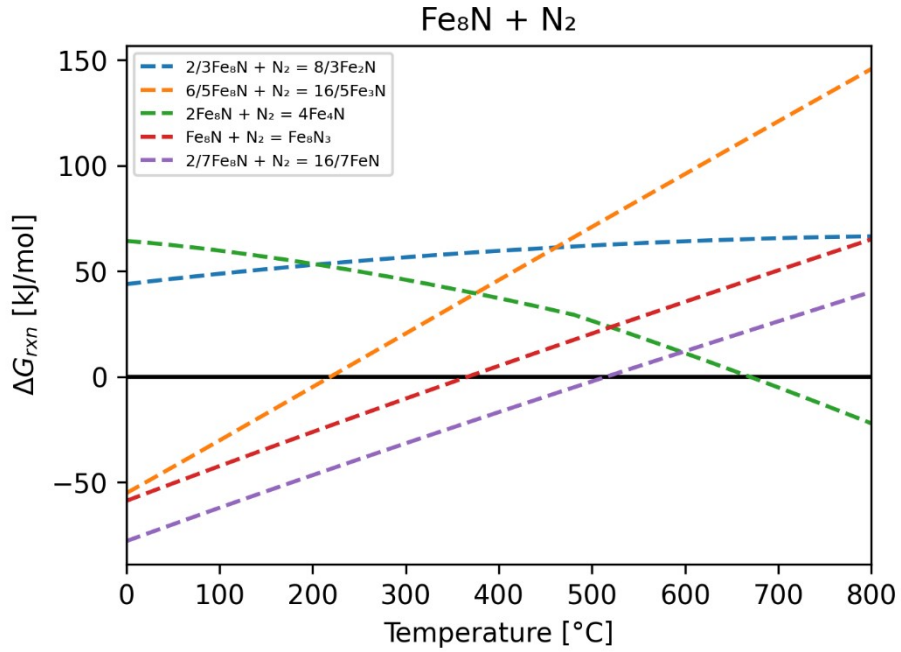

Figure S50: Ellingham diagram of the Fe_8N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

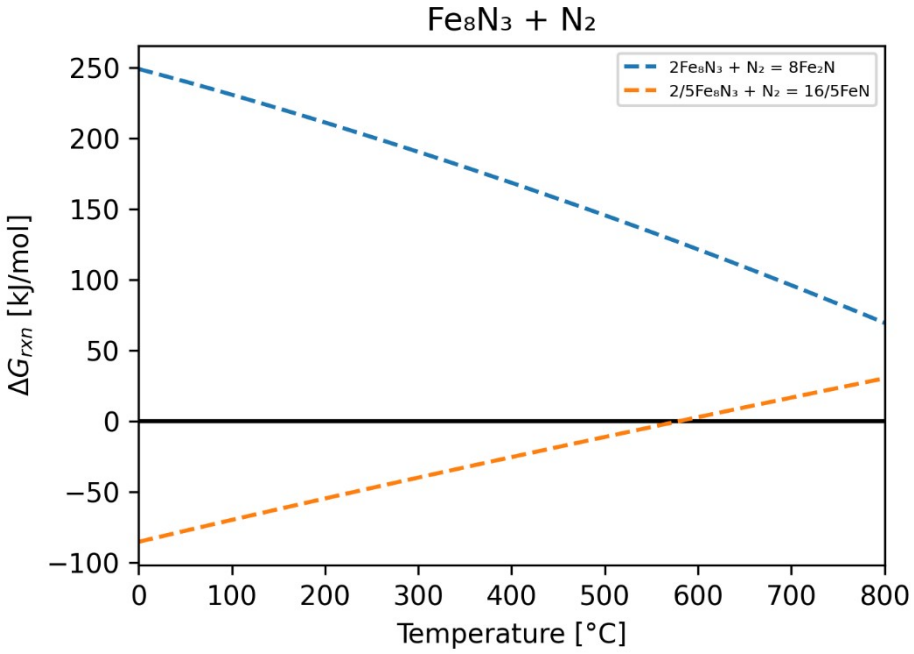

Figure S51: Ellingham diagram of the Fe_8N_3 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

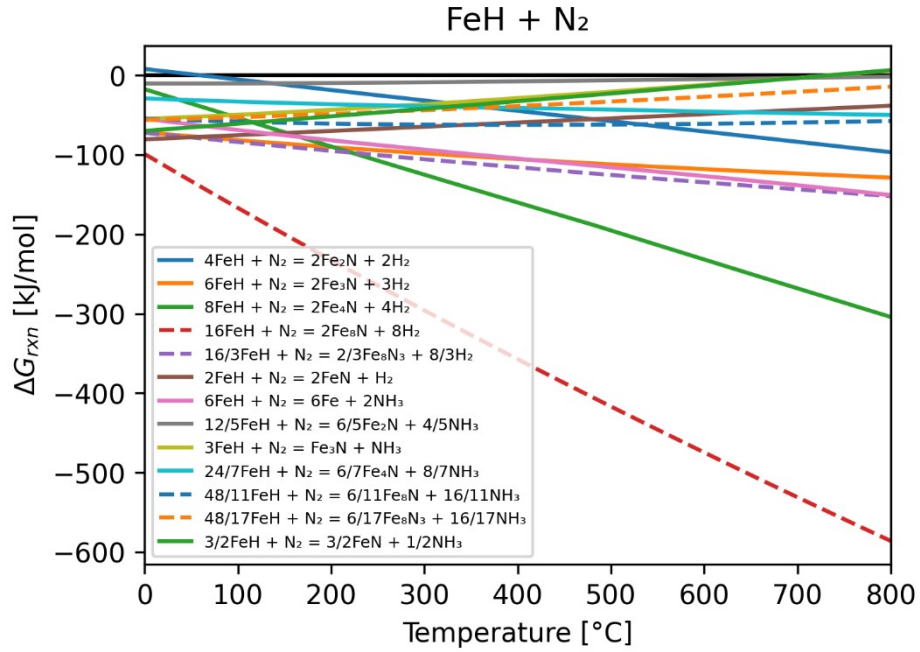

Figure S52: Ellingham diagram of the FeH nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

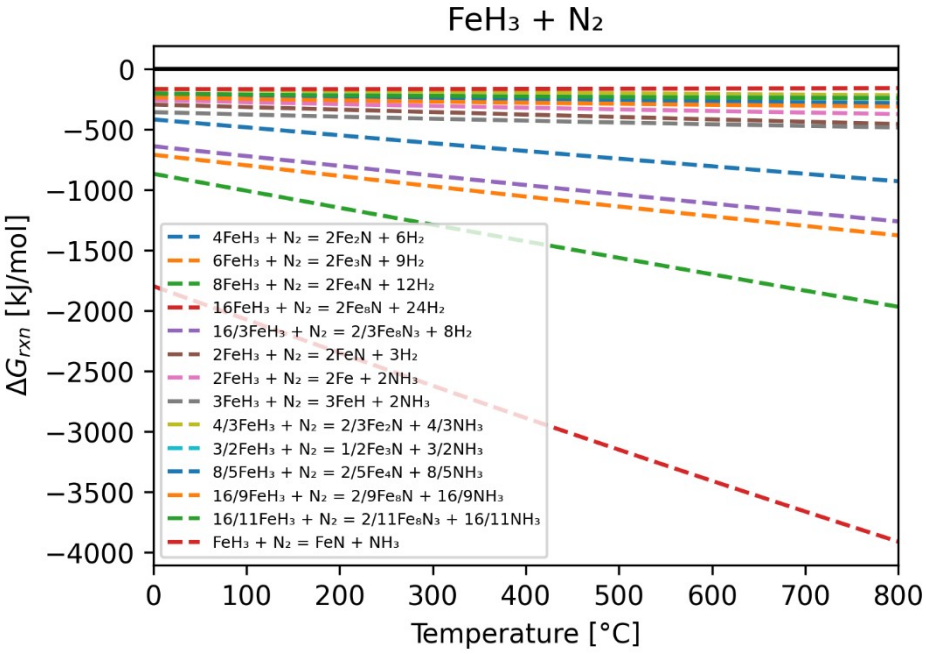

Figure S53: Ellingham diagram of the FeH_3 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

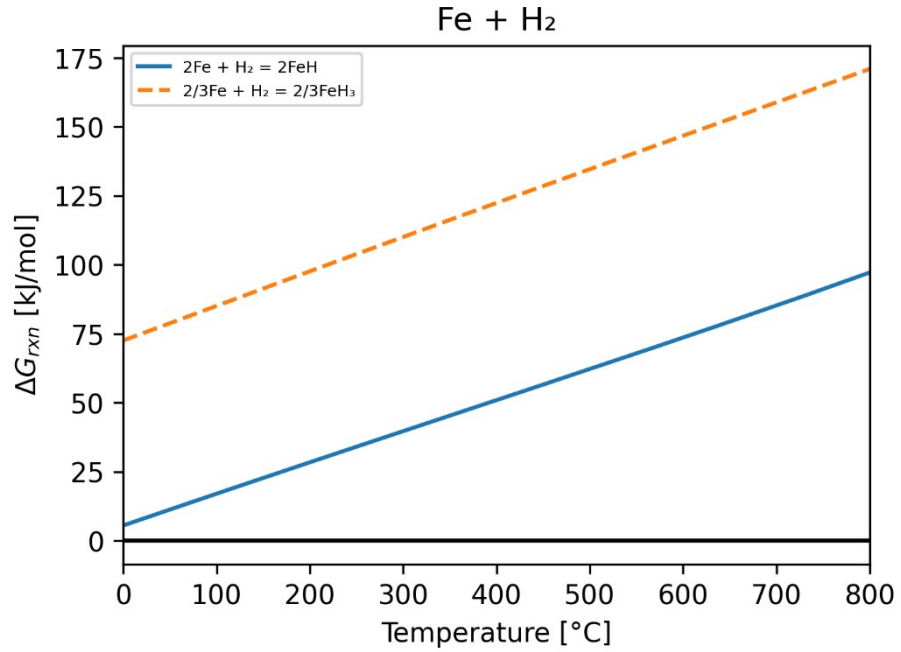

Figure S54: Ellingham diagram of the Fe hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

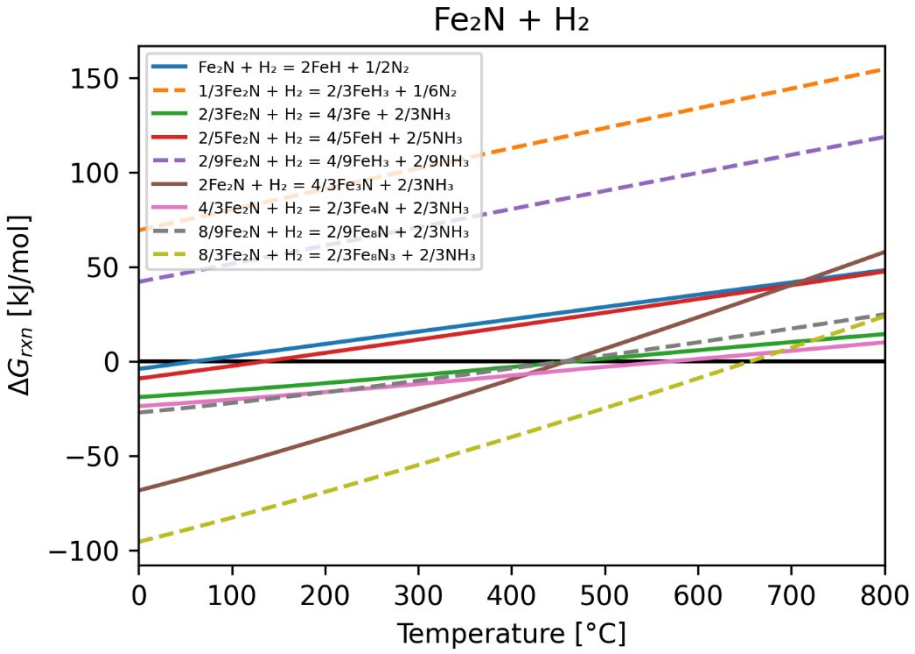

Figure S55: Ellingham diagram of the Fe_2N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

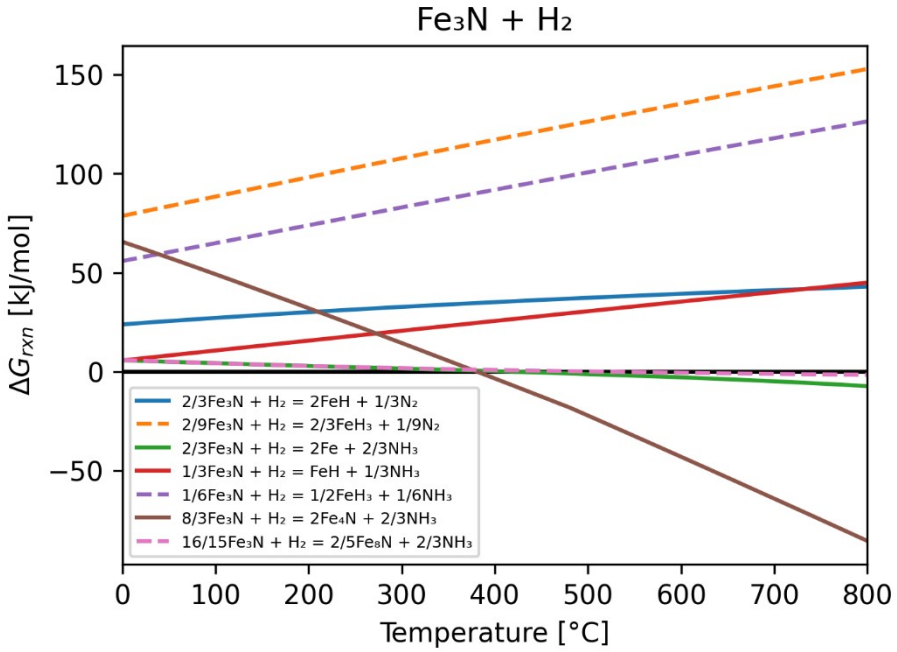

Figure S56: Ellingham diagram of the Fe_3N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

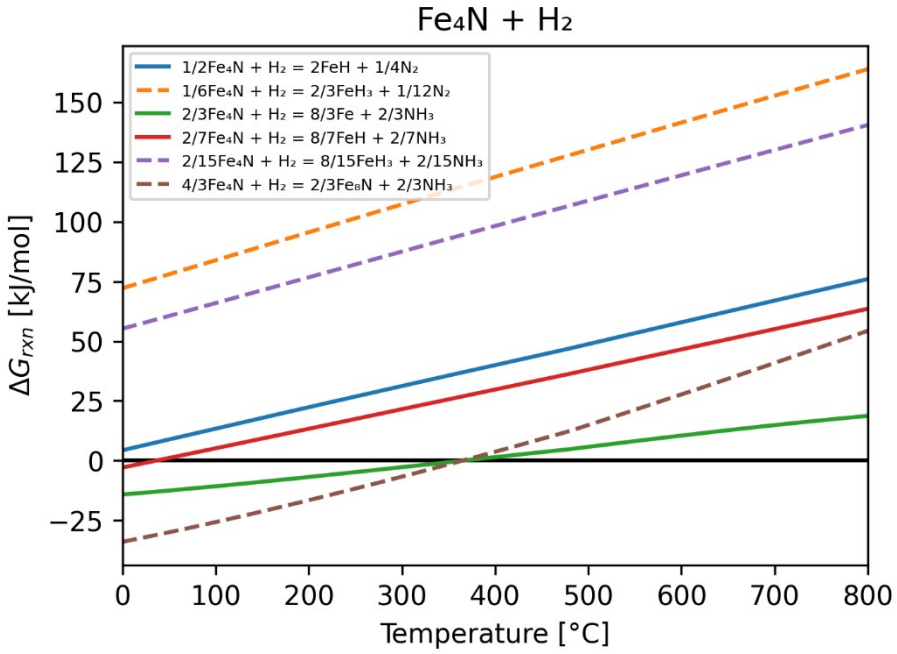

Figure S57: Ellingham diagram of the Fe_4N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

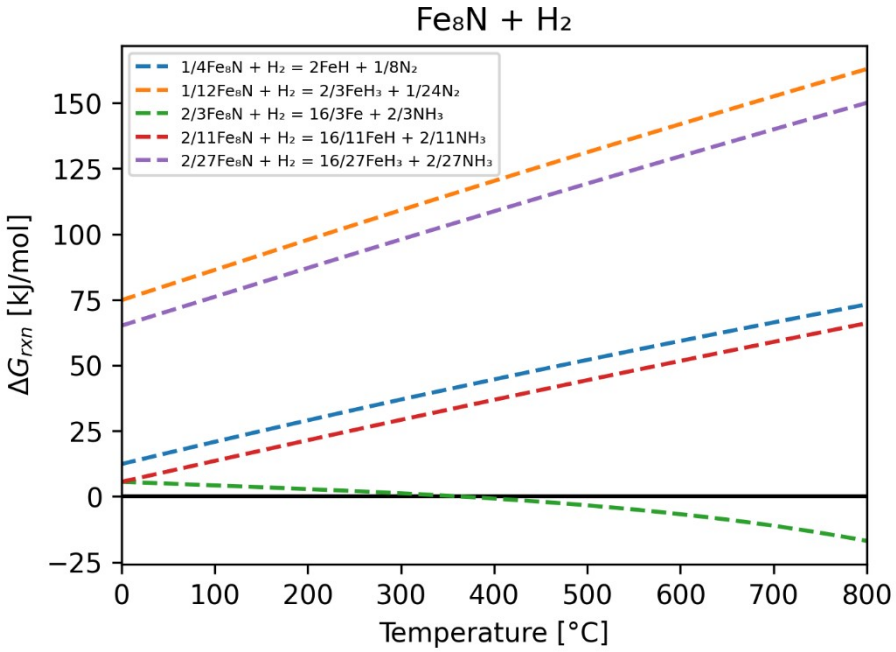

Figure S58: Ellingham diagram of the Fe8N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

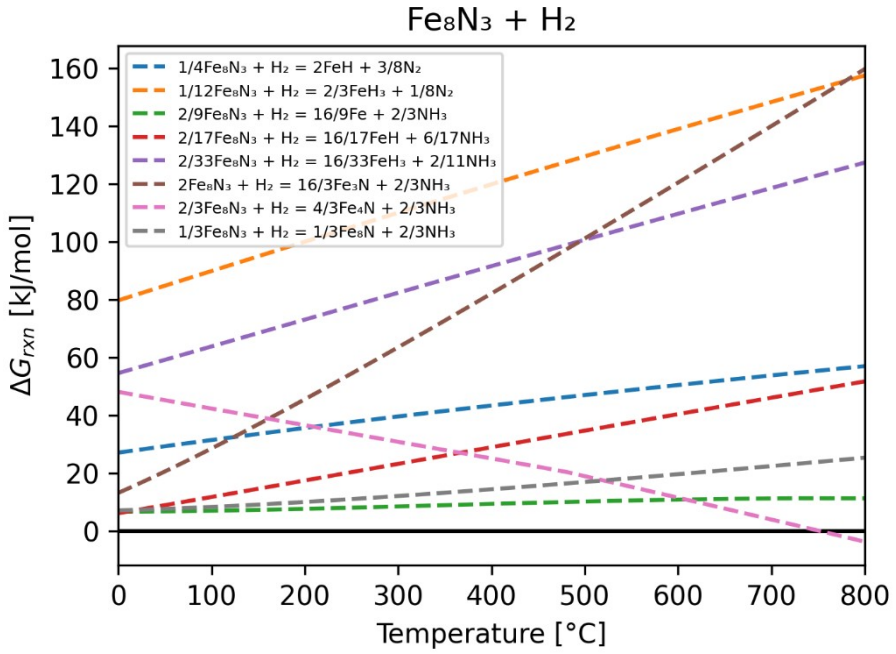

Figure S59: Ellingham diagram of the Fe_8N_3 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

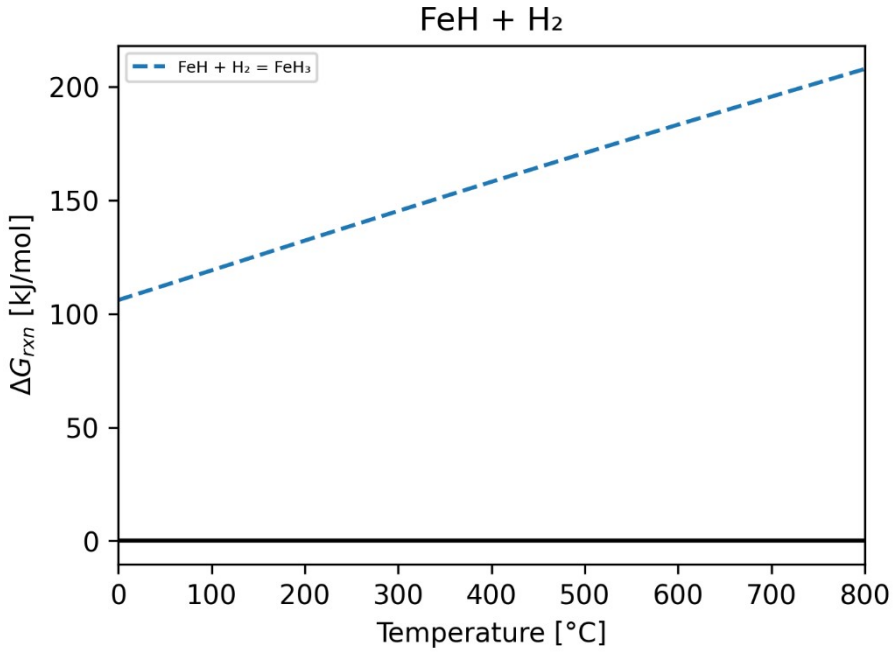

Figure S60: Ellingham diagram of the FeH hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

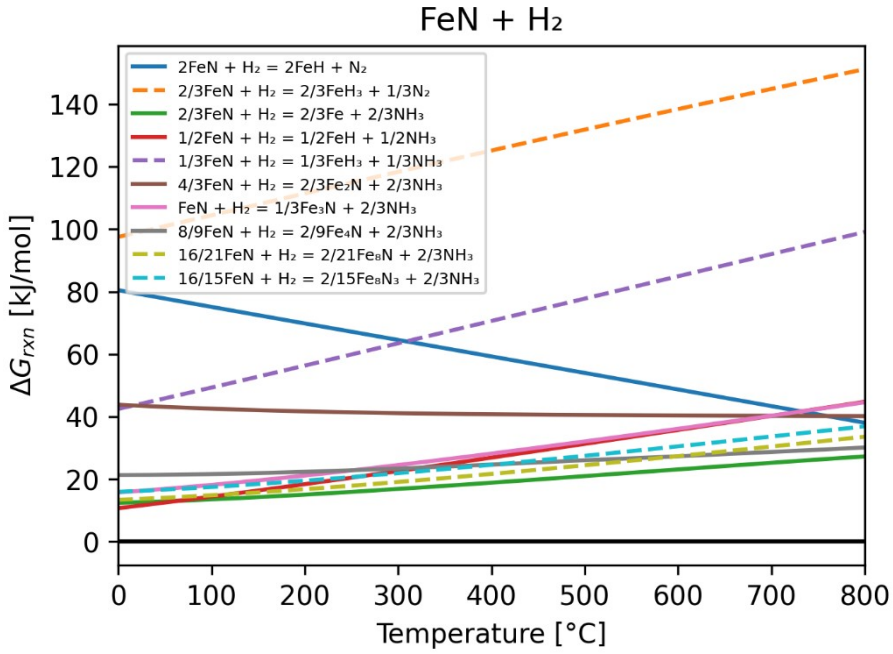

Figure S61: Ellingham diagram of the FeN hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

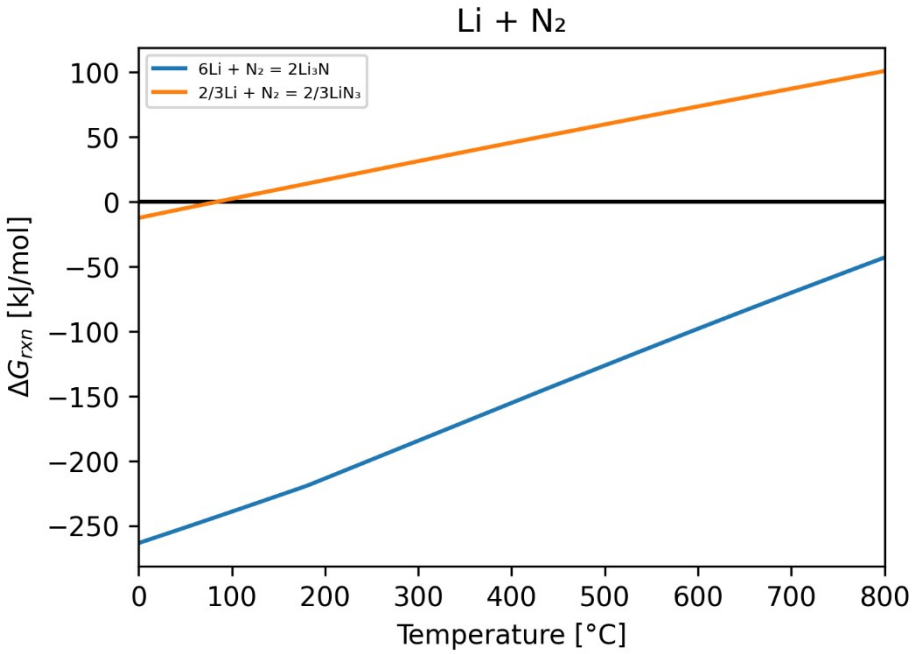

Figure S62: Ellingham diagram of the Li nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

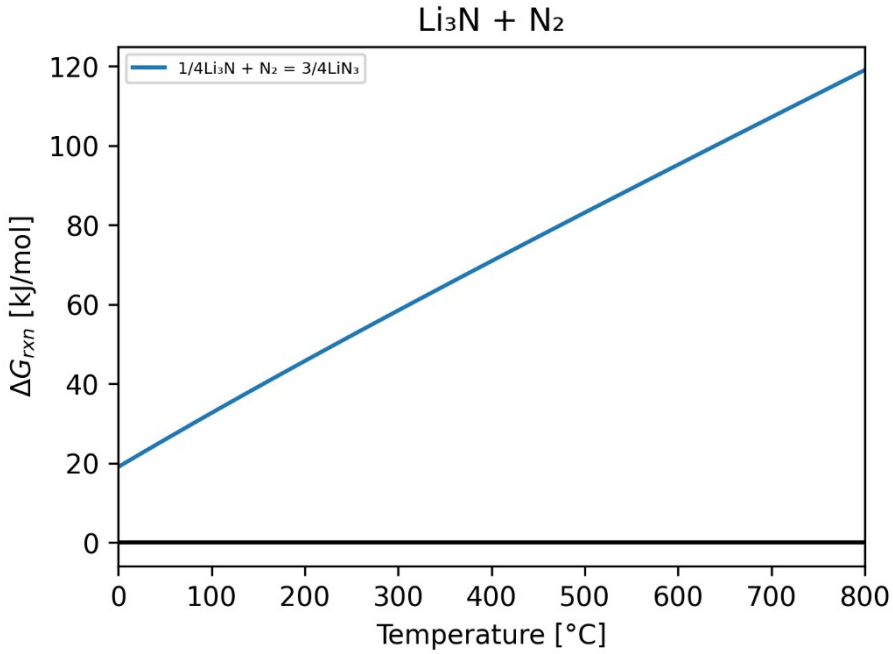

Figure S63: Ellingham diagram of the Li_3N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

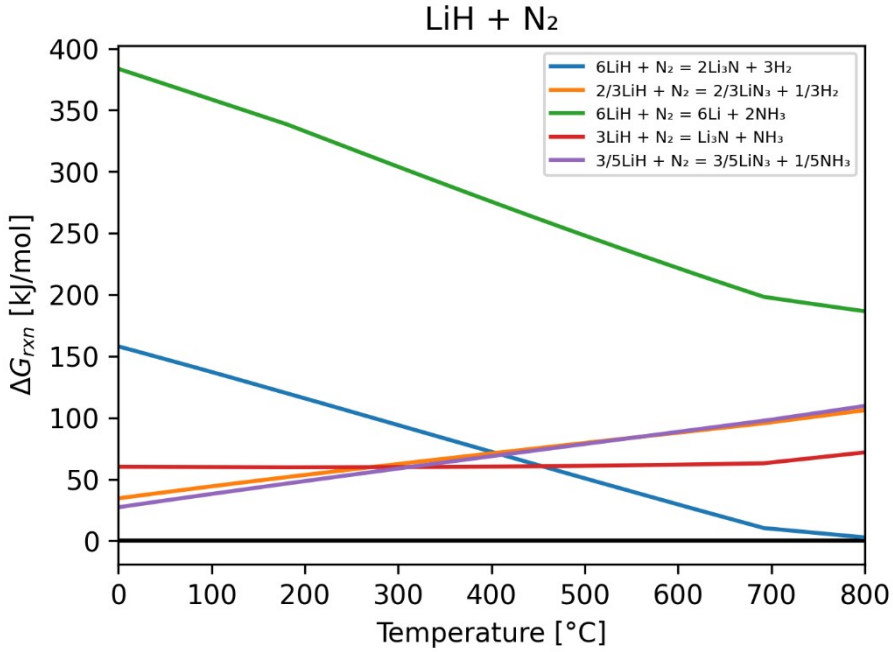

Figure S64: Ellingham diagram of the LiH nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

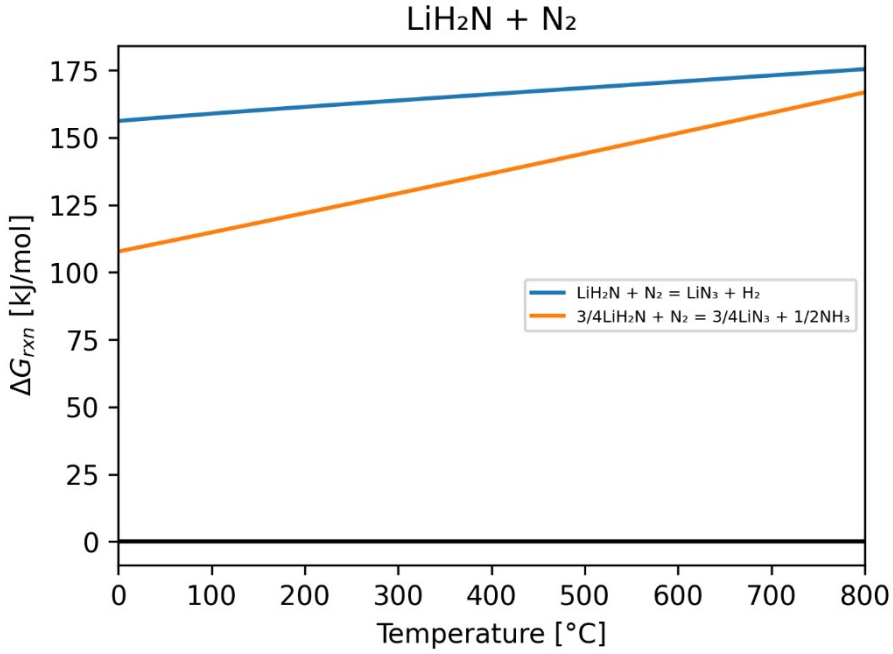

Figure S65: Ellingham diagram of the LiH_2N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

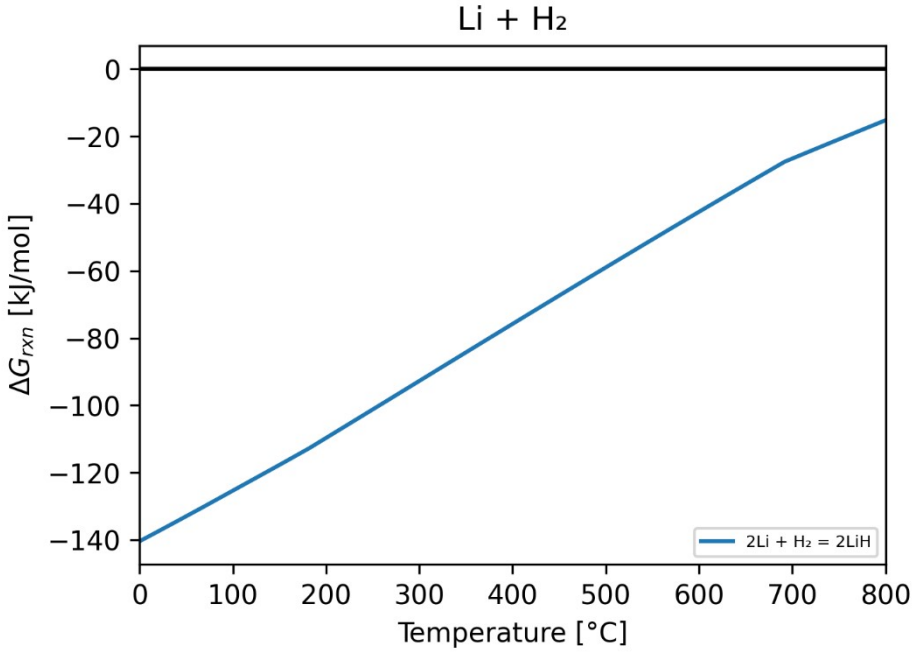

Figure S66: Ellingham diagram of the Li hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

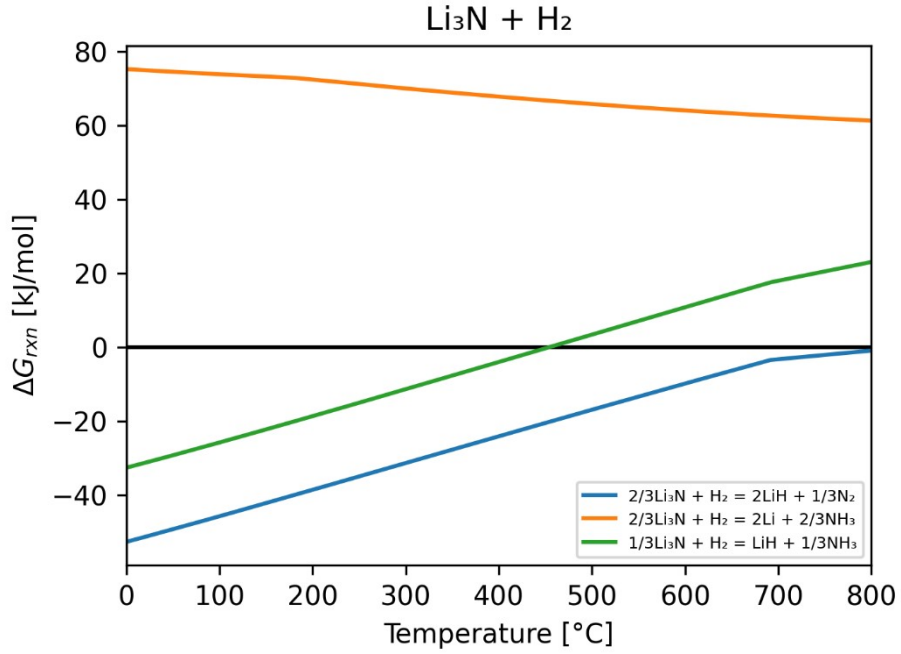

Figure S67: Ellingham diagram of the Li_3N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

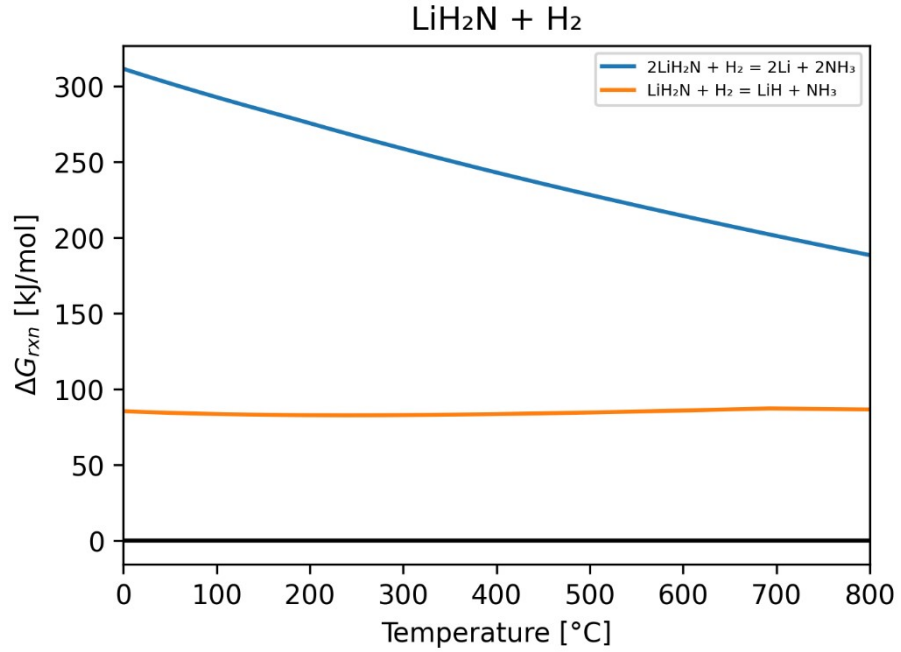

Figure S68: Ellingham diagram of the LiH_2N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

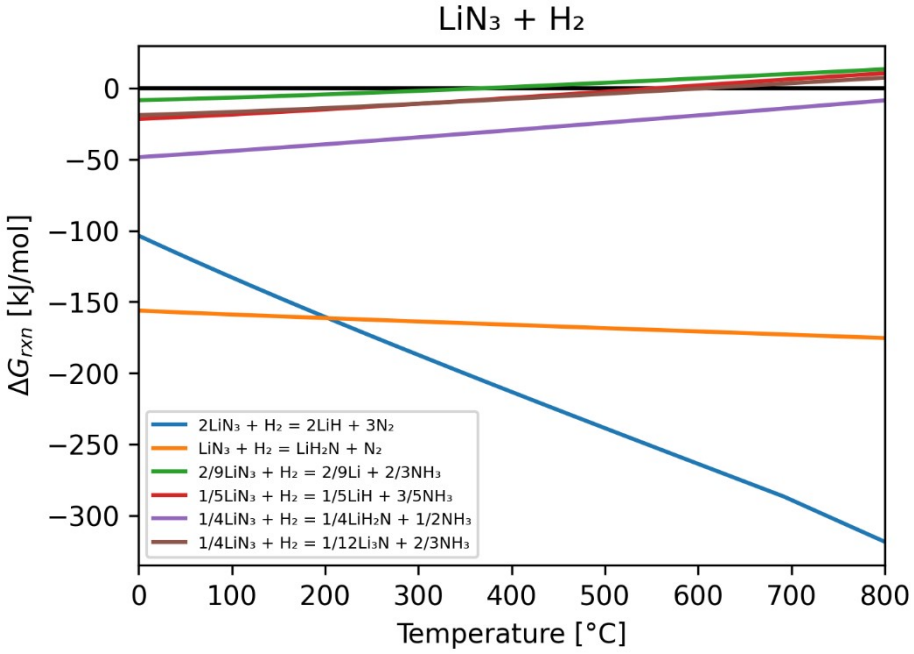

Figure S69: Ellingham diagram of the LiN_3 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

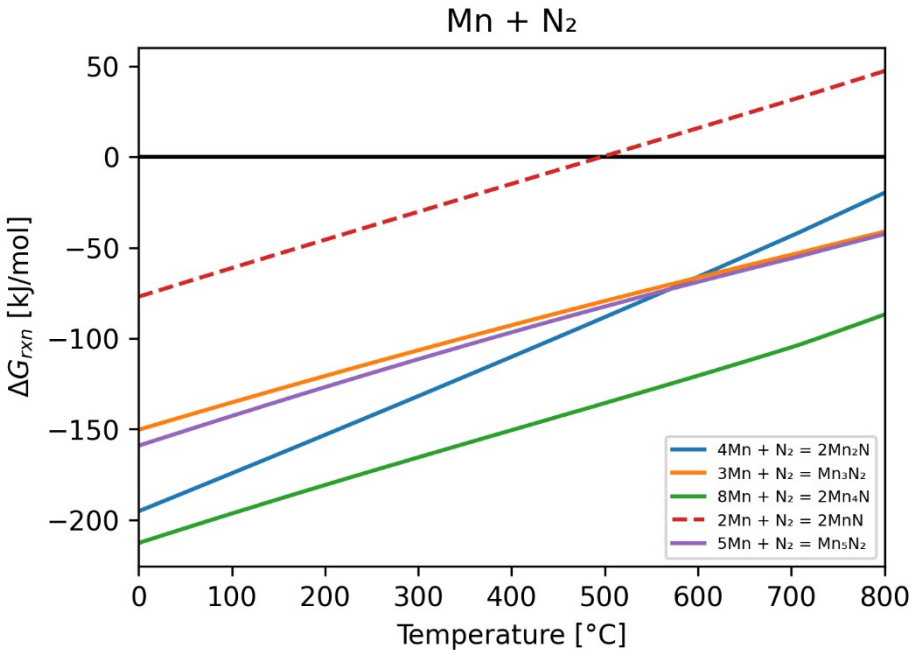

Figure S70: Ellingham diagram of the Mn nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

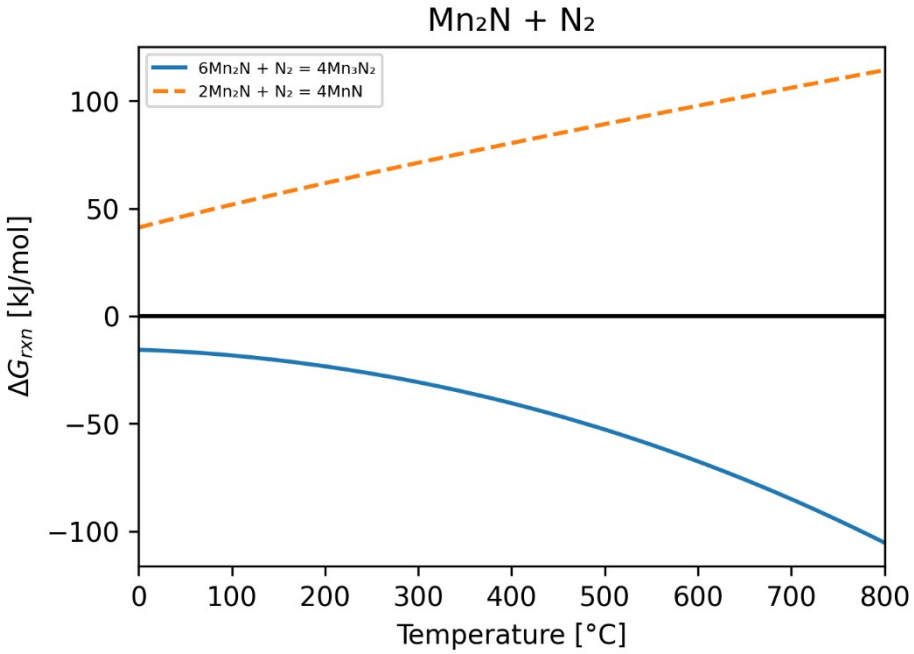

Figure S71: Ellingham diagram of the Mn_2N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

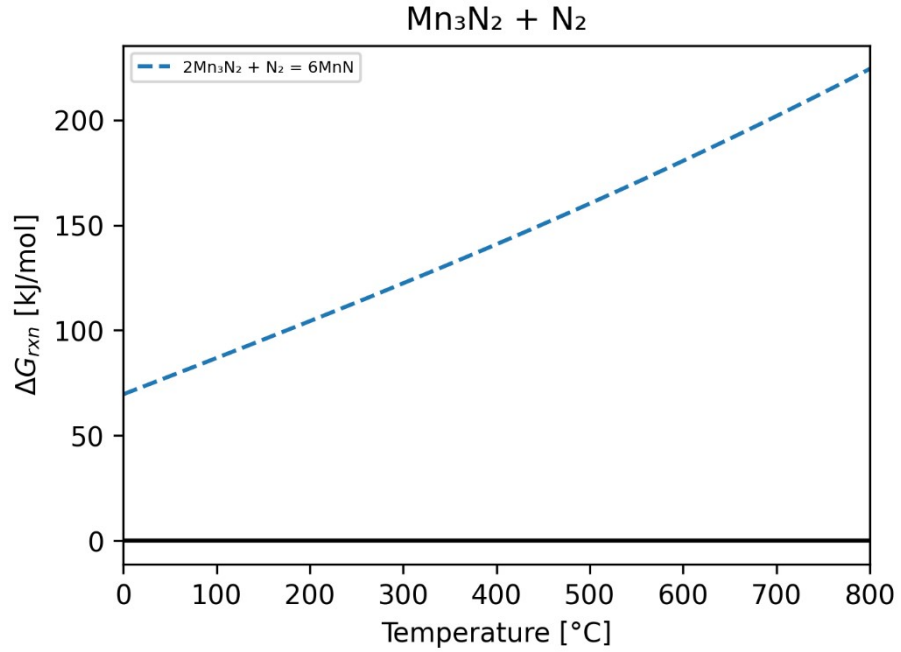

Figure S72: Ellingham diagram of the Mn_3N_2 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

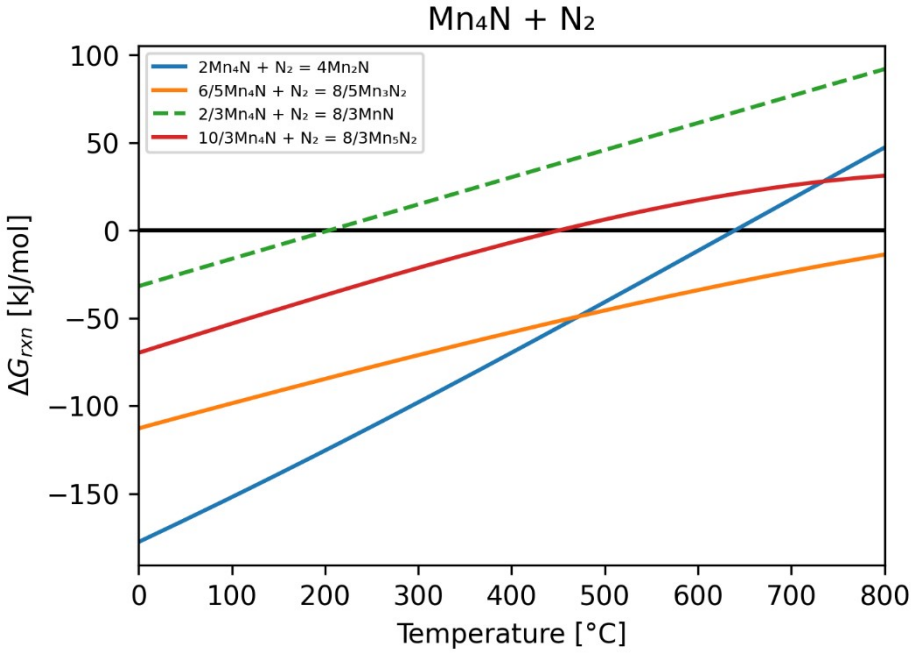

Figure S73: Ellingham diagram of the Mn_4N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

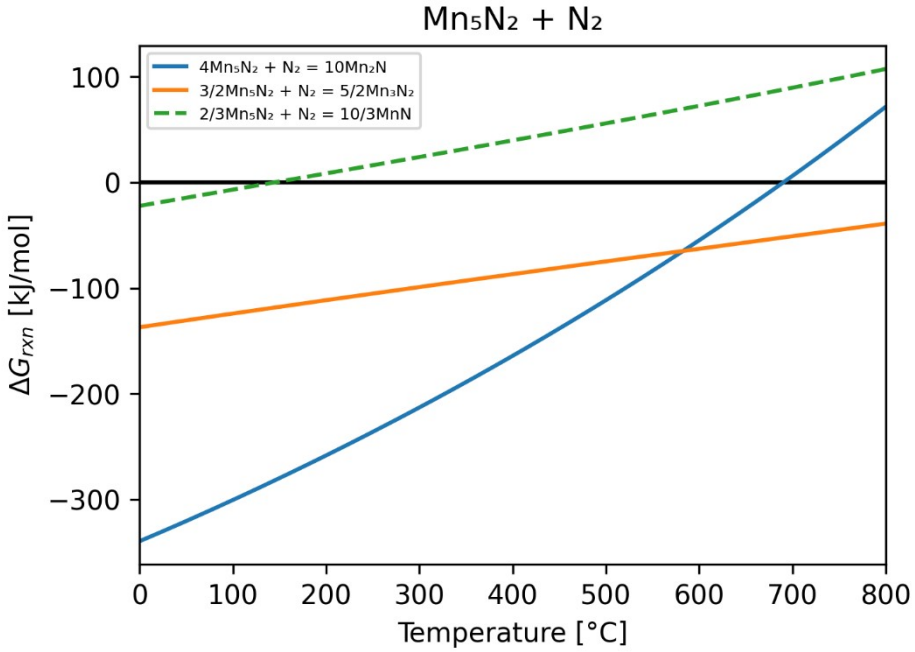

Figure S74: Ellingham diagram of the Mn_5N_2 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

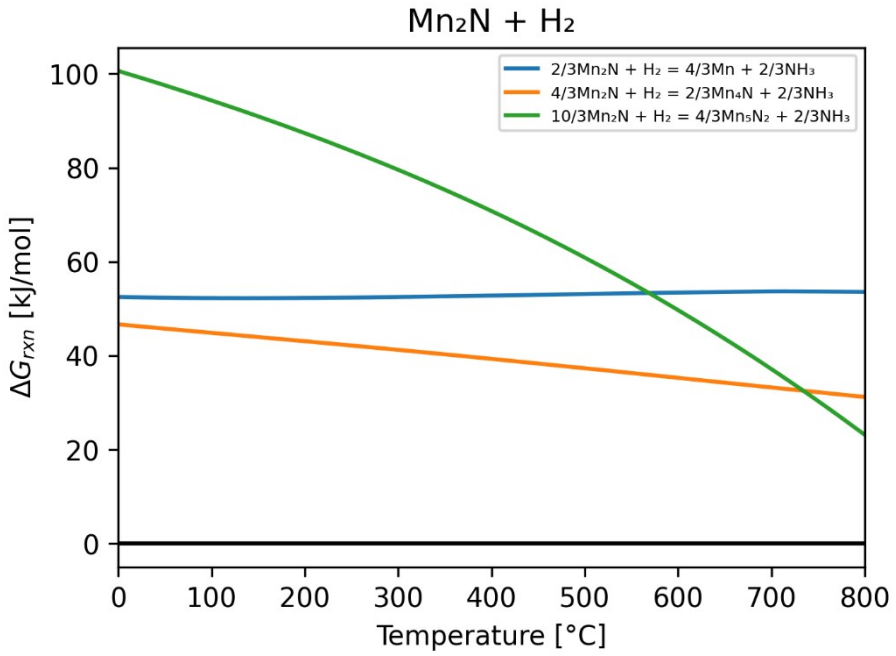

Figure S75: Ellingham diagram of the Mn_2N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

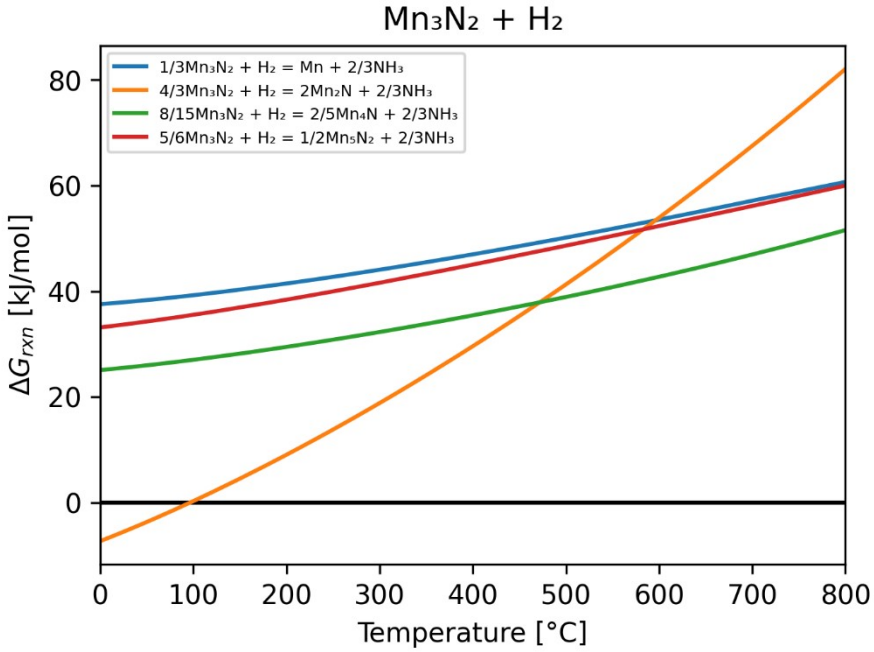

Figure S76: Ellingham diagram of the Mn_3N_2 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

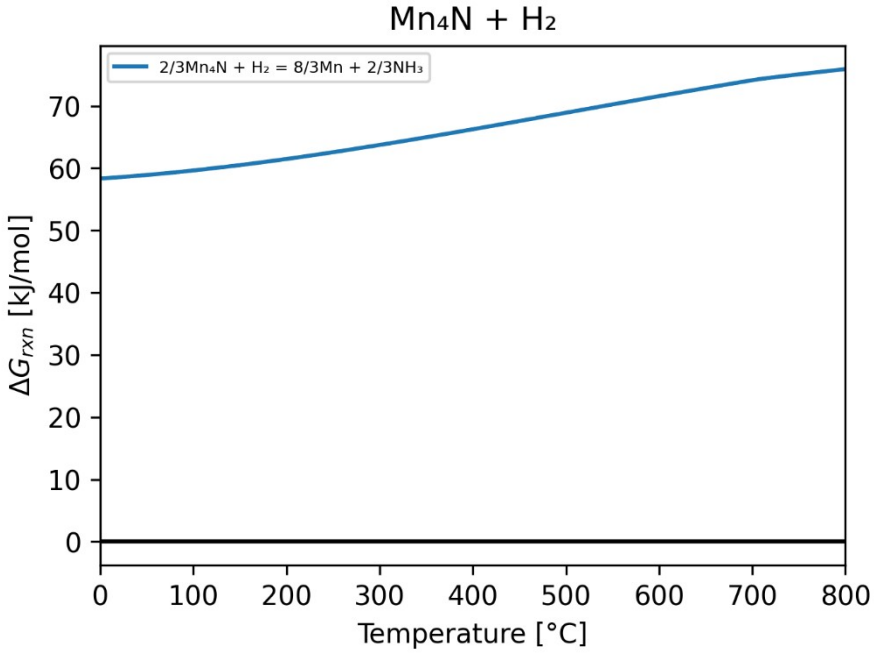

Figure S77: Ellingham diagram of the Mn_4N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

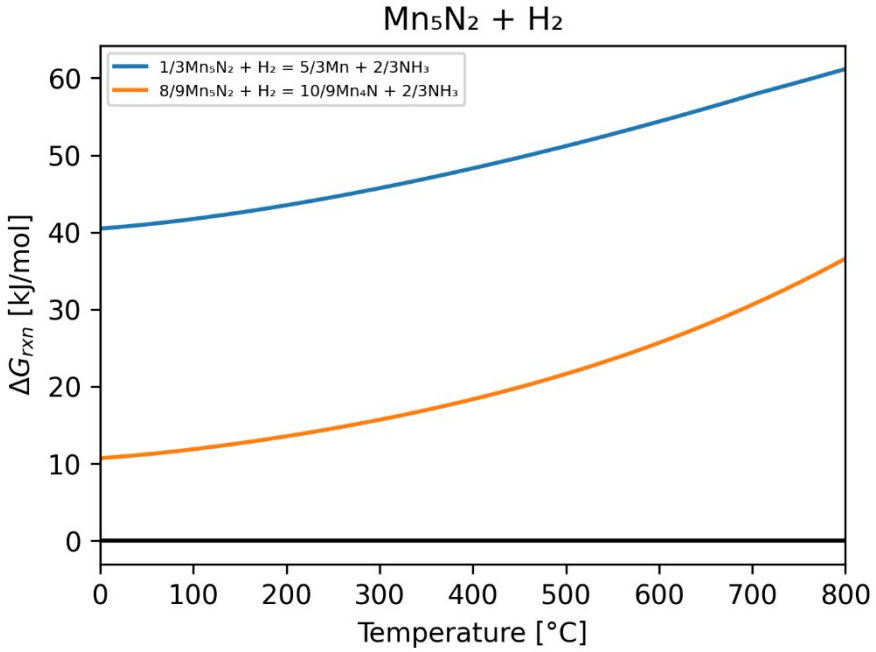

Figure S78: Ellingham diagram of the Mn_5N_2 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

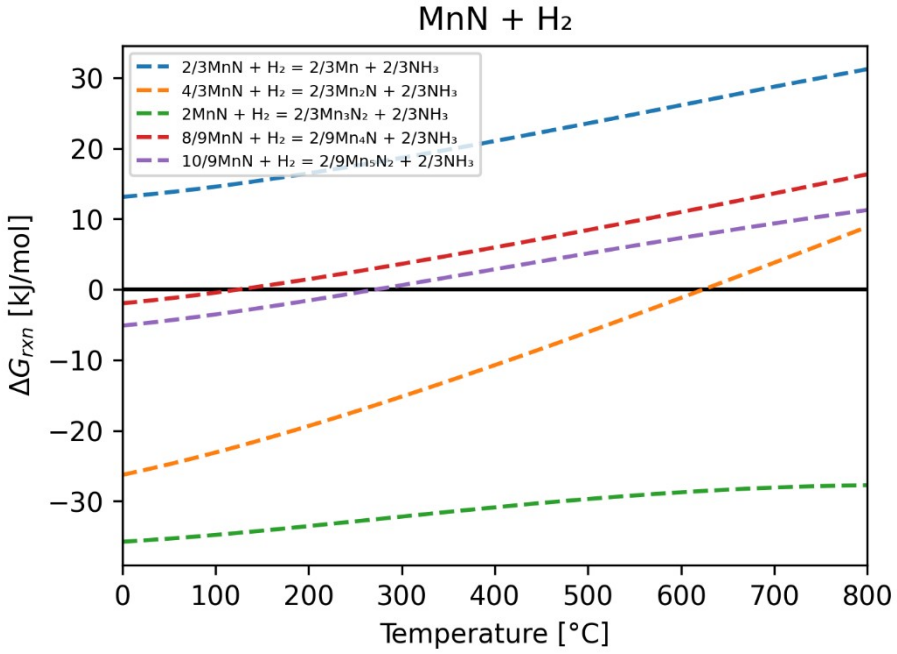

Figure S79: Ellingham diagram of the MnN hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

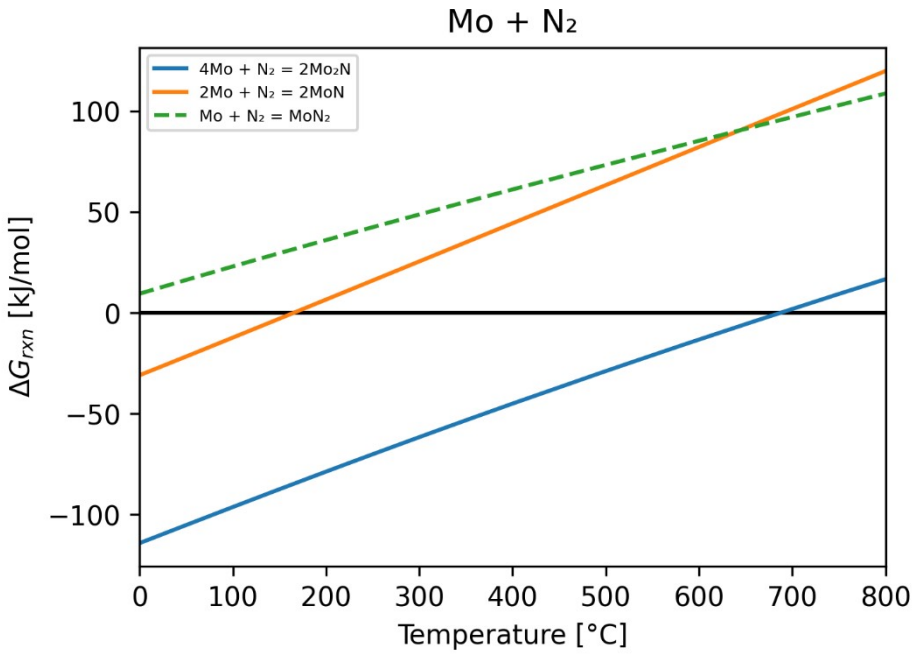

Figure S80: Ellingham diagram of the Mo nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

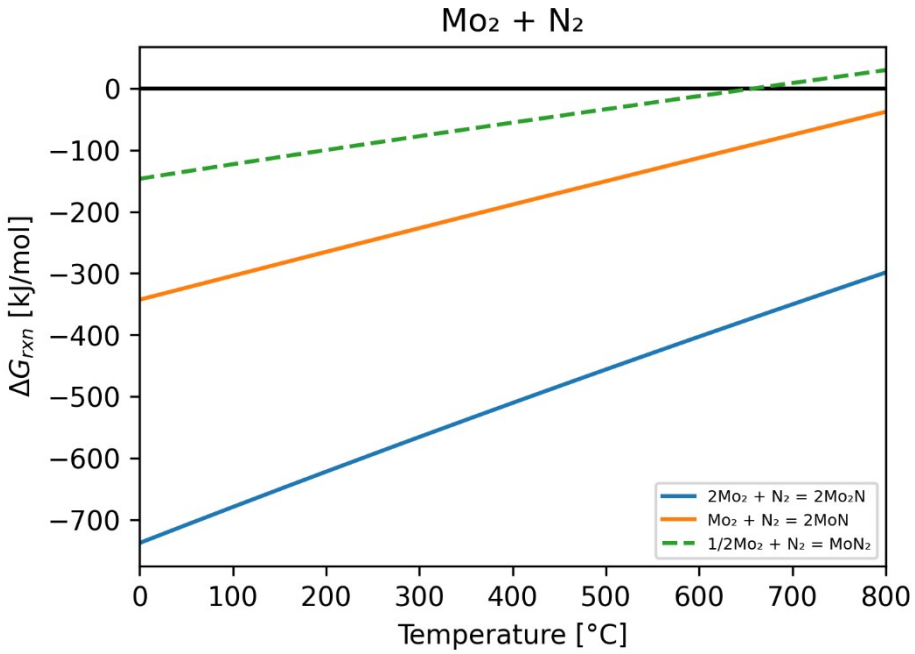

Figure S81: Ellingham diagram of the Mo_2 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

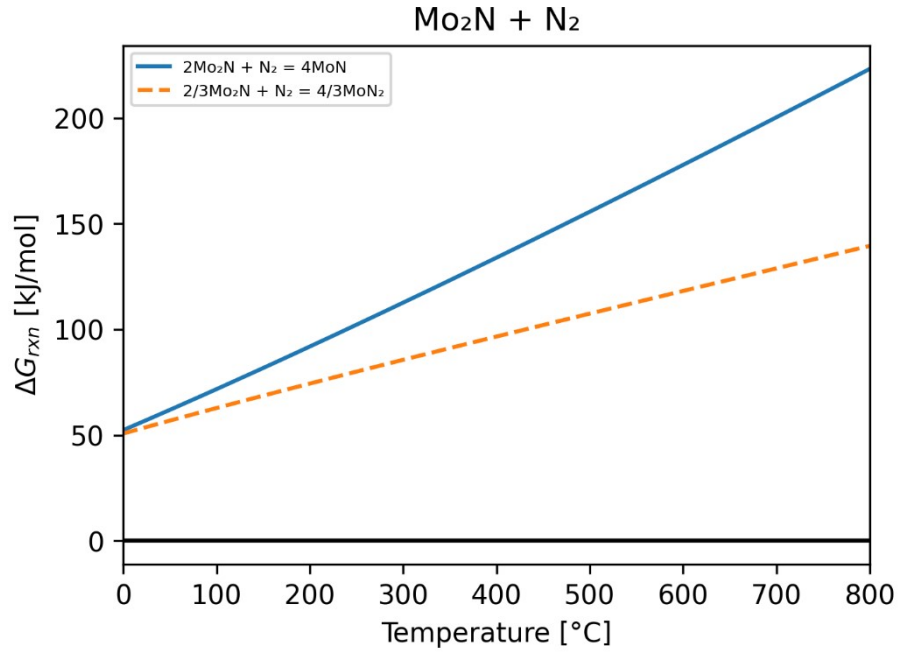

Figure S82: Ellingham diagram of the Mo_2N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

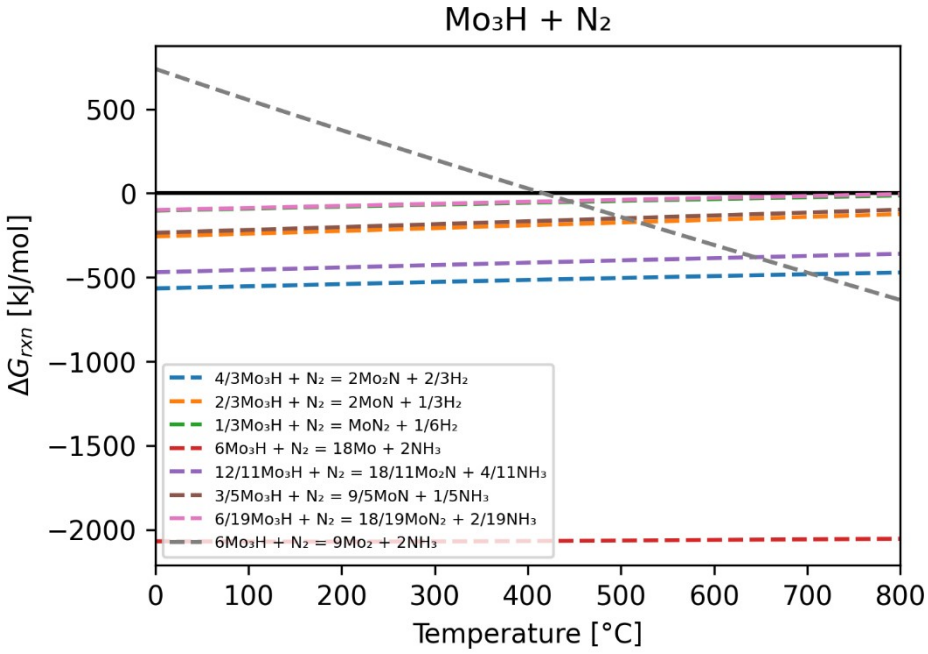

Figure S83: Ellingham diagram of the Mo_3H nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

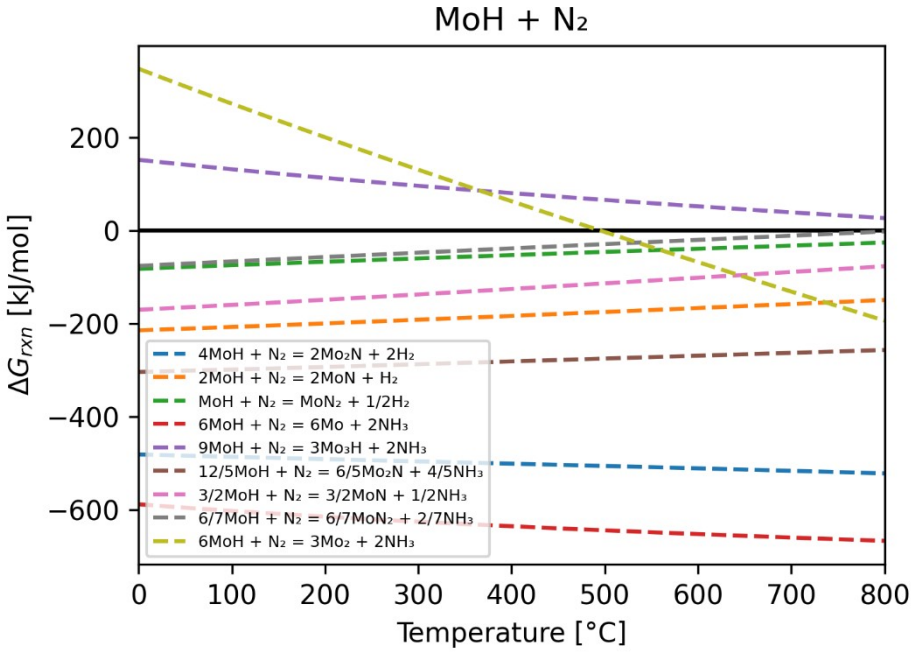

Figure S84: Ellingham diagram of the MoH nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

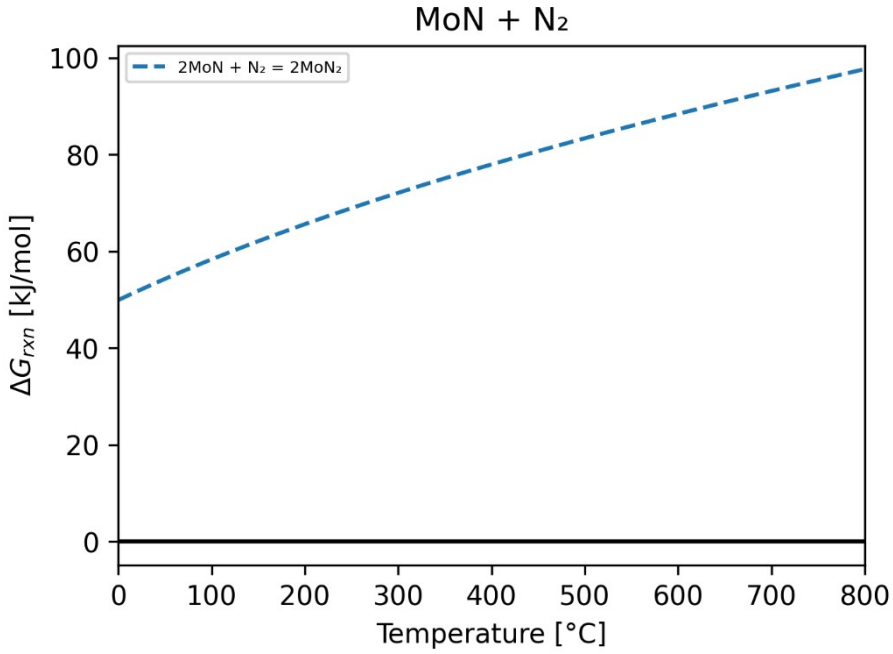

Figure S85: Ellingham diagram of the MoN nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

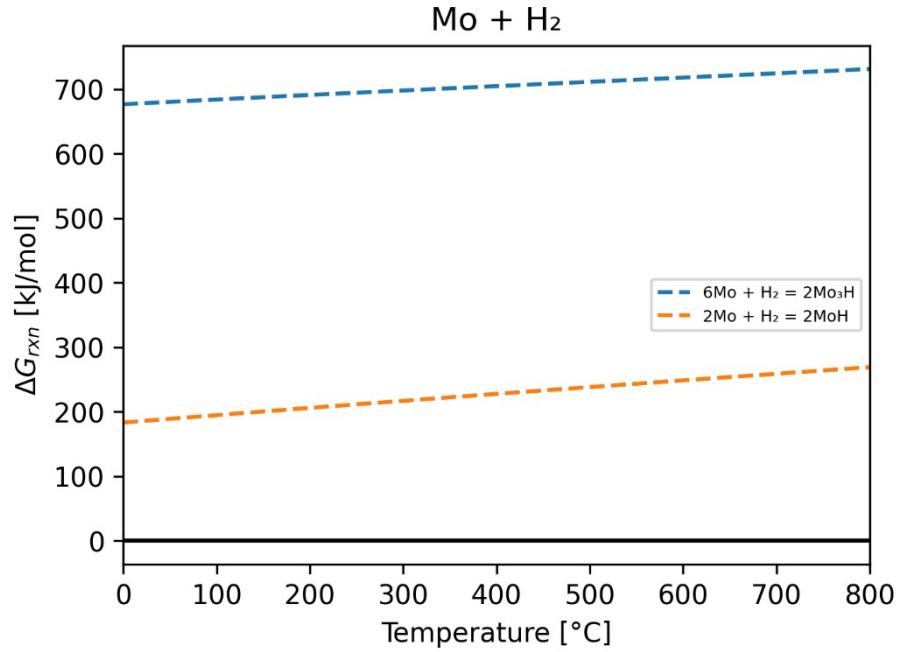

Figure S86: Ellingham diagram of the Mo hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

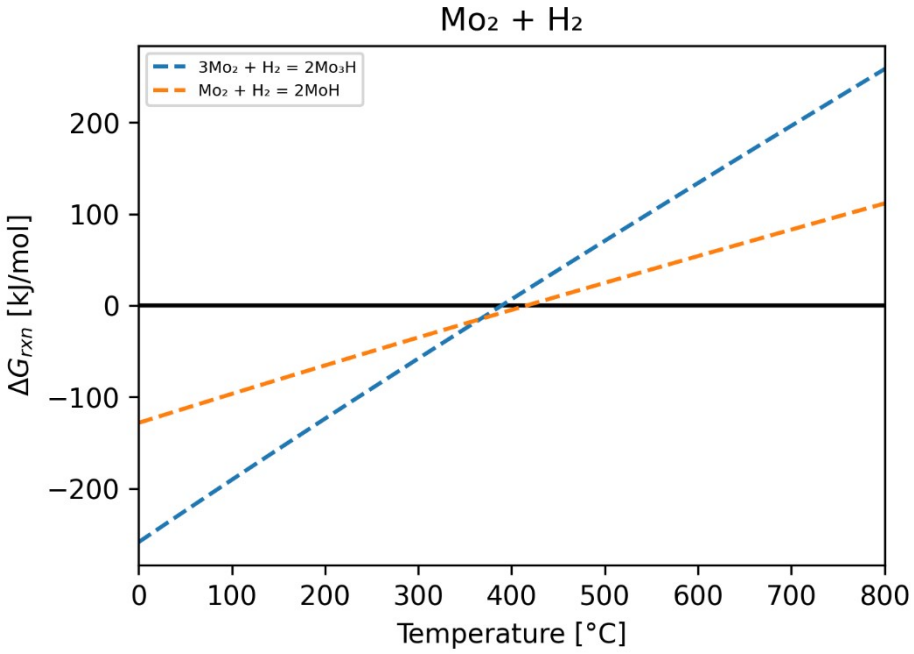

Figure S87: Ellingham diagram of the Mo_2 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

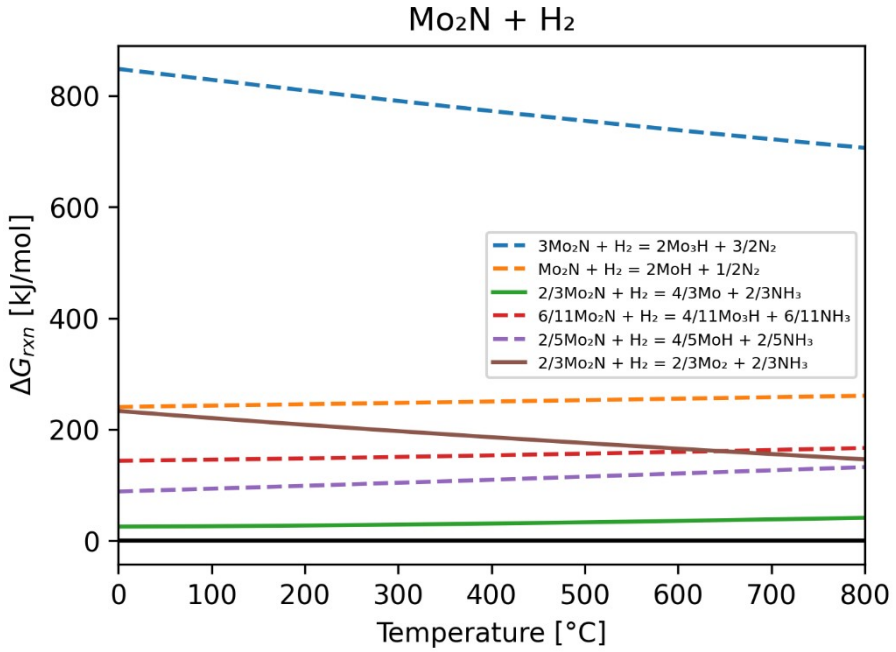

Figure S88: Ellingham diagram of the Mo_2N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

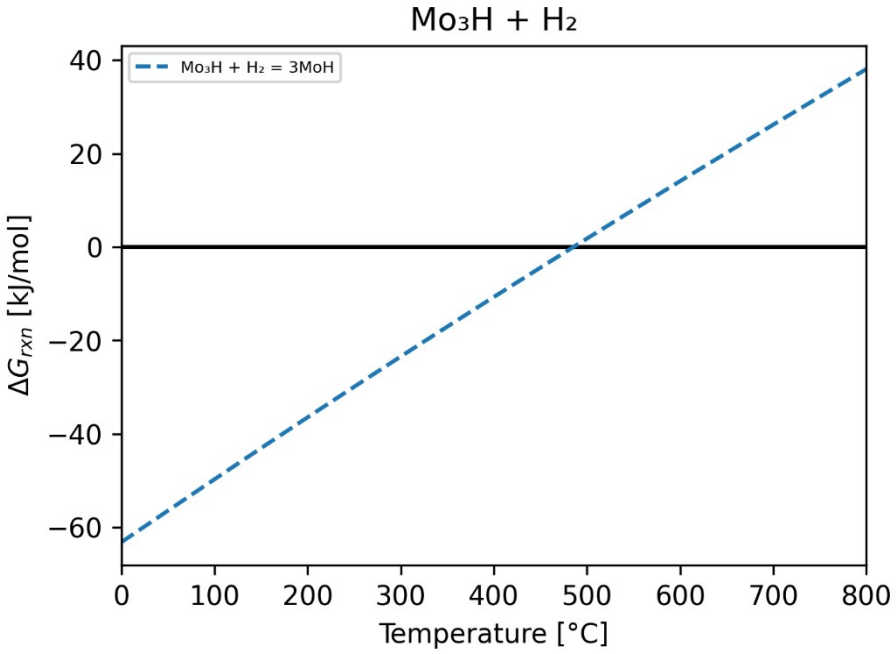

Figure S89: Ellingham diagram of the Mo_3H hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

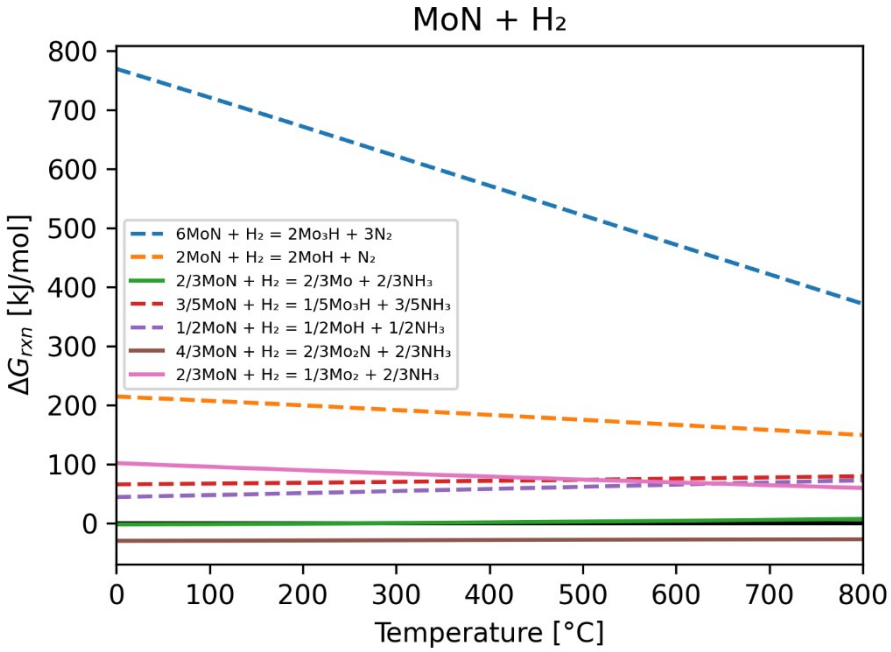

Figure S90: Ellingham diagram of the MoN hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

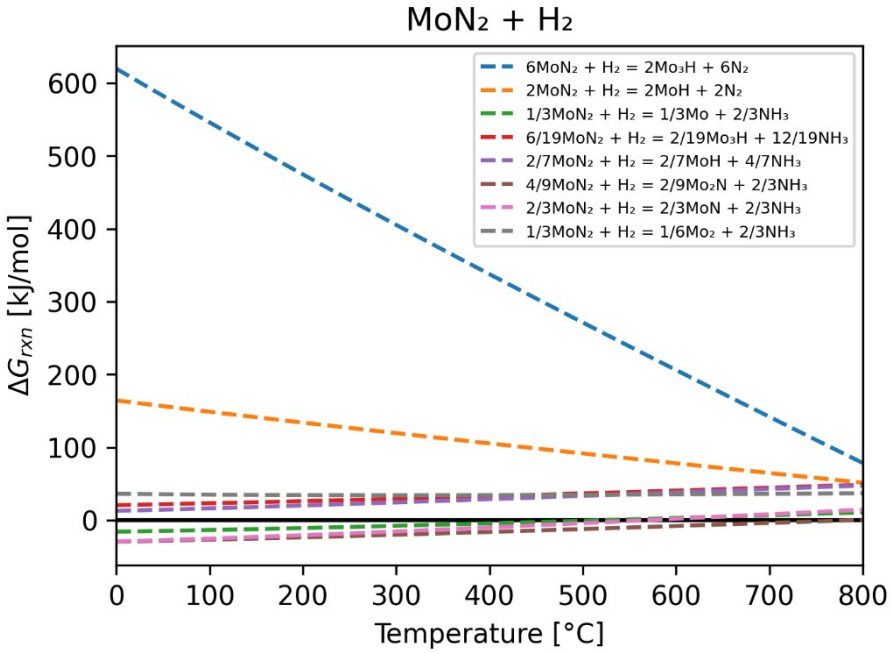

Figure S91: Ellingham diagram of the MoN_2 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

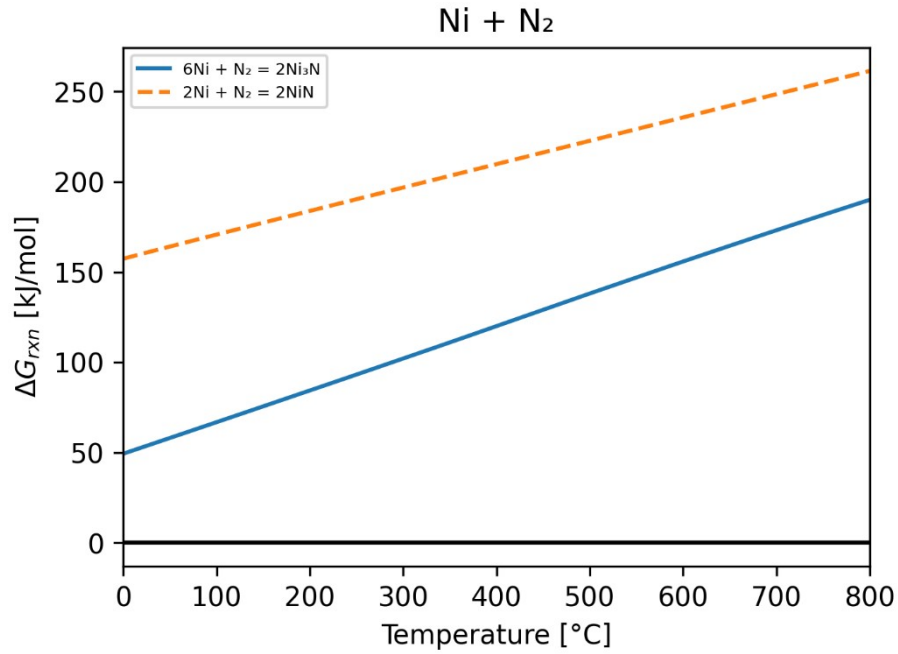

Figure S92: Ellingham diagram of the Ni nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

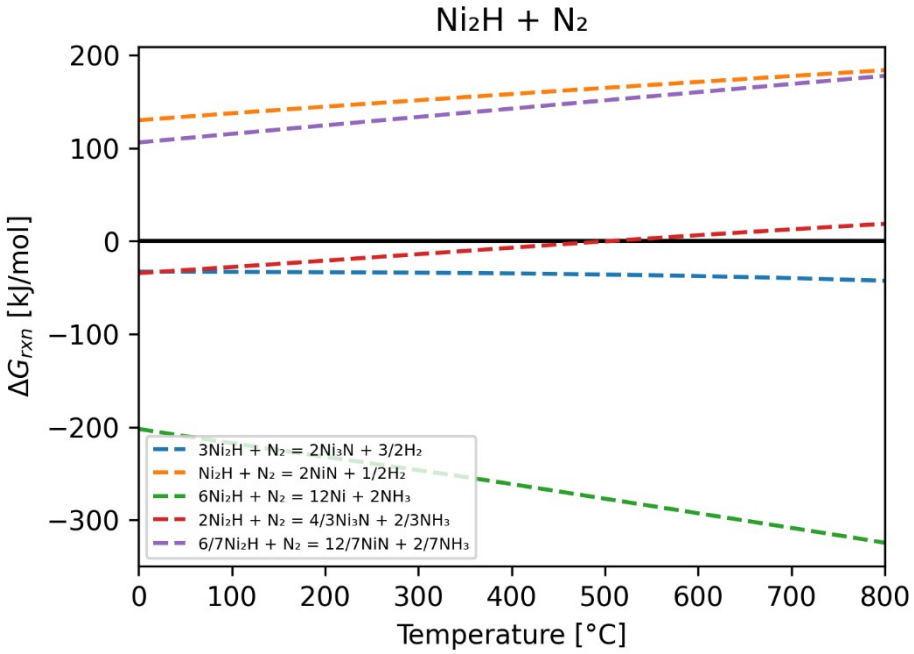

Figure S93: Ellingham diagram of the Ni_2H nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

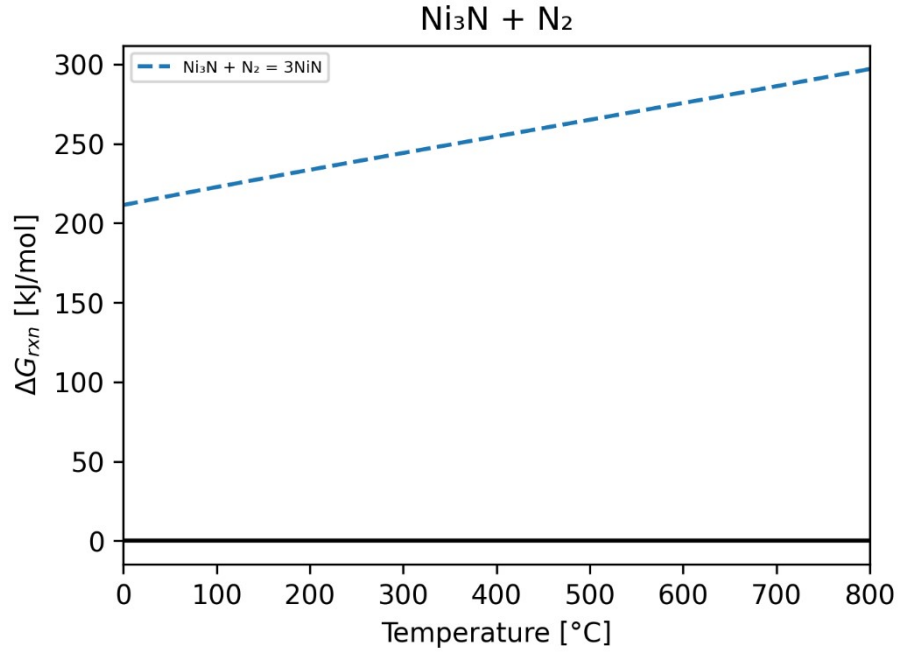

Figure S94: Ellingham diagram of the Ni_3N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

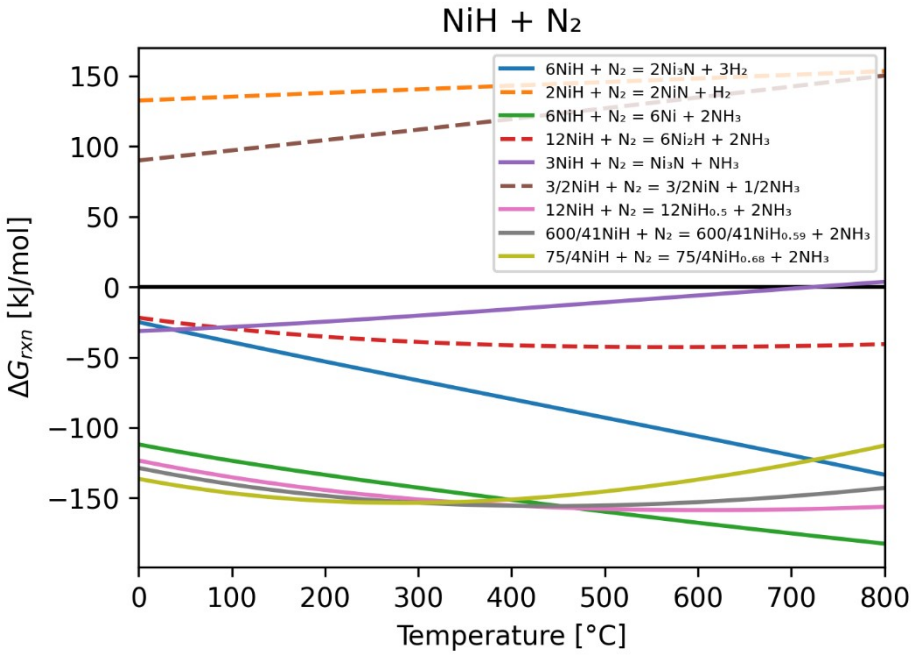

Figure S95: Ellingham diagram of the NiH nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

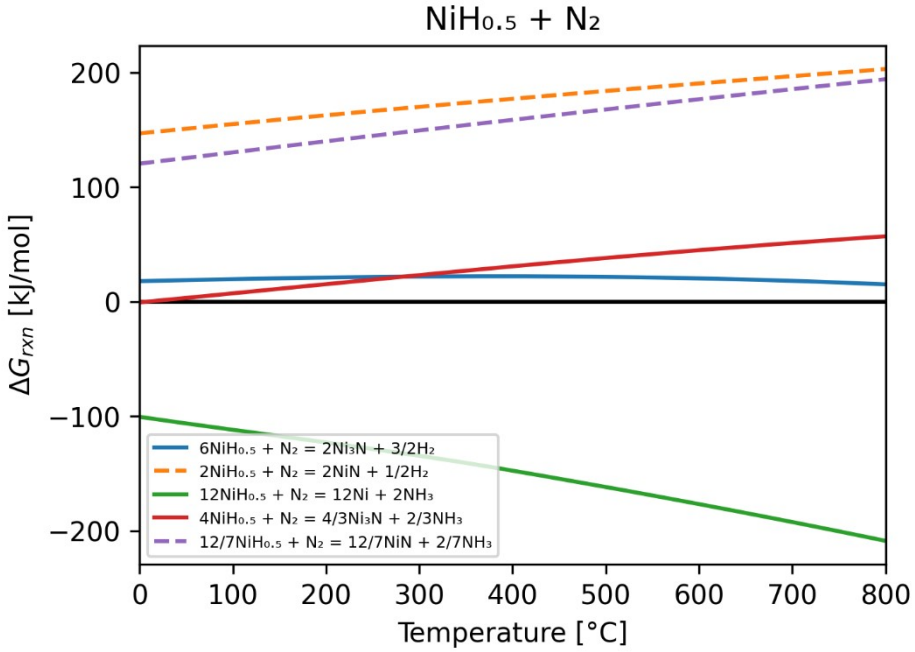

Figure S96: Ellingham diagram of the $NiH_{0.5}$ nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

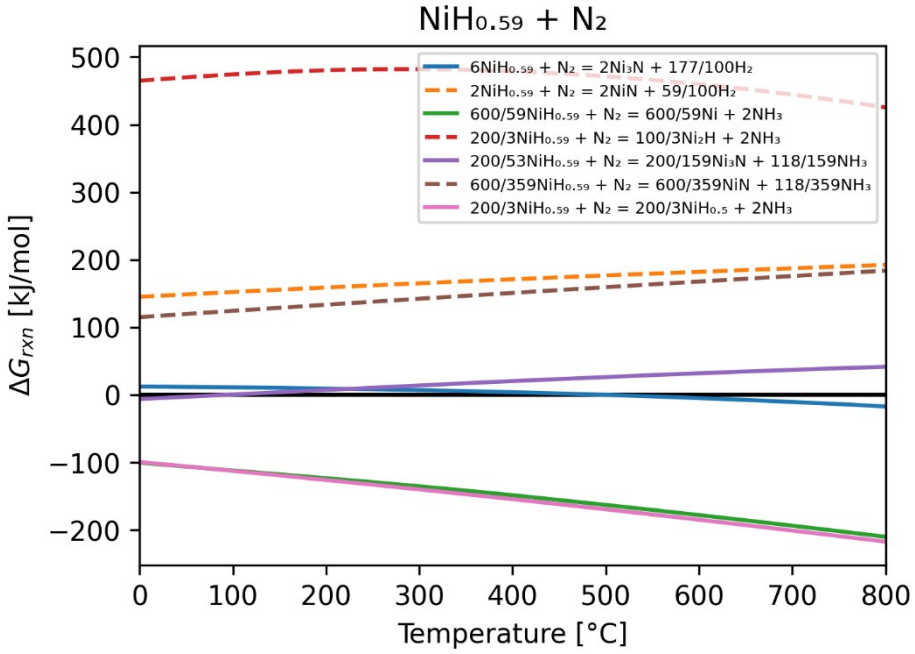

Figure S97: Ellingham diagram of the $NiH_{0.59}$ nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

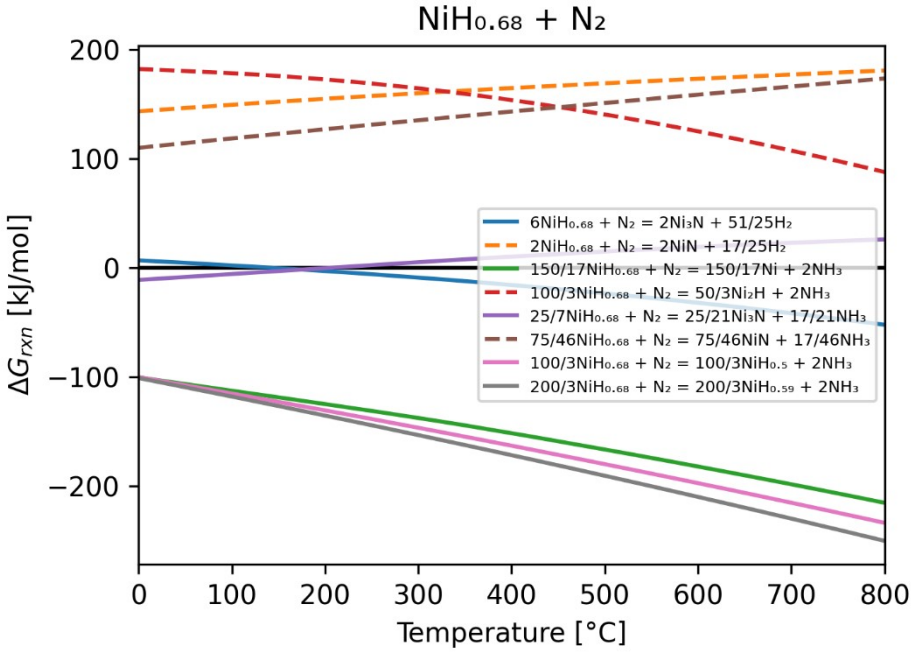

Figure S98: Ellingham diagram of the $NiH_{0.68}$ nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

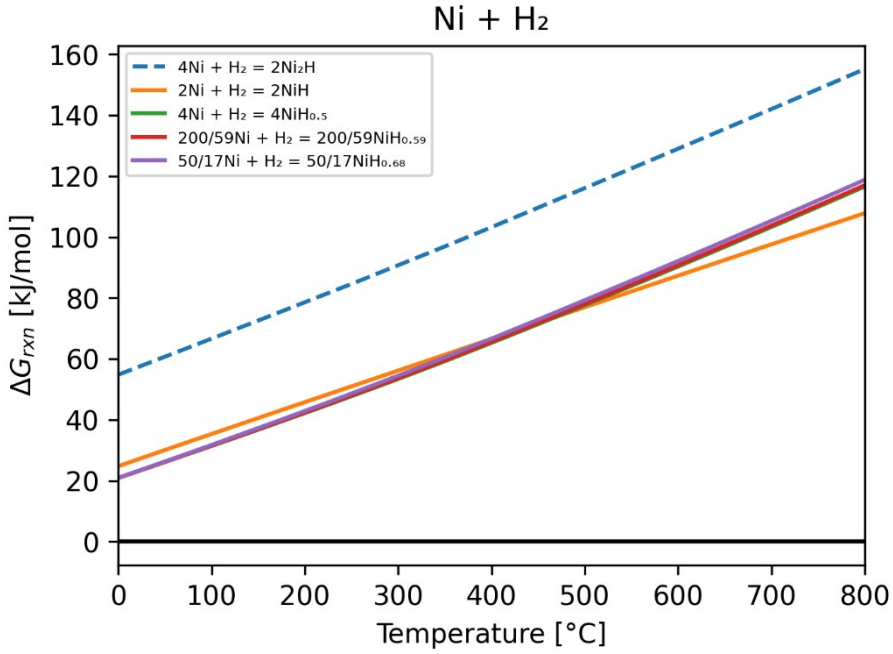

Figure S99: Ellingham diagram of the Ni hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

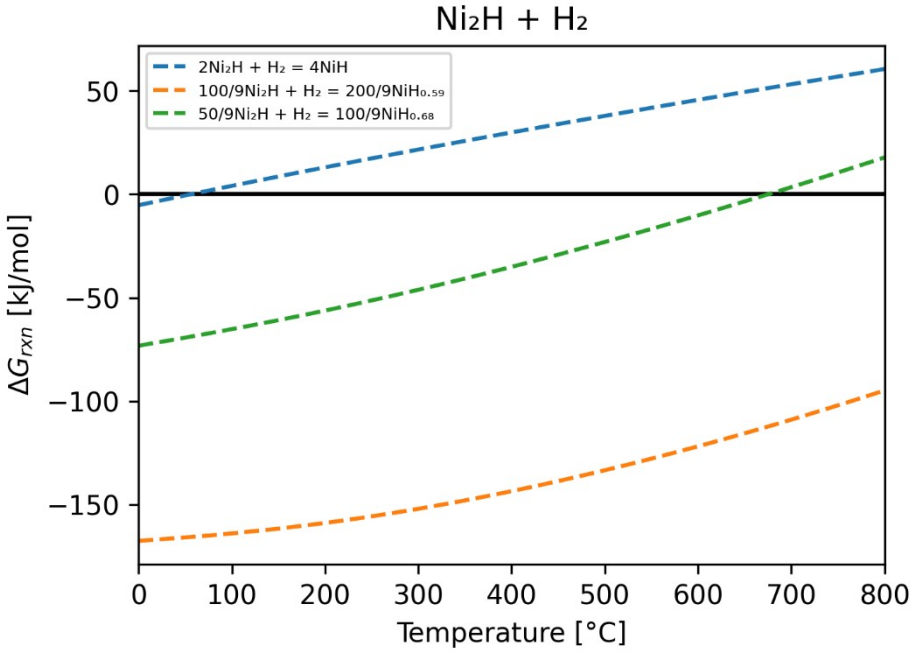

Figure S100: Ellingham diagram of the Ni_2H hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

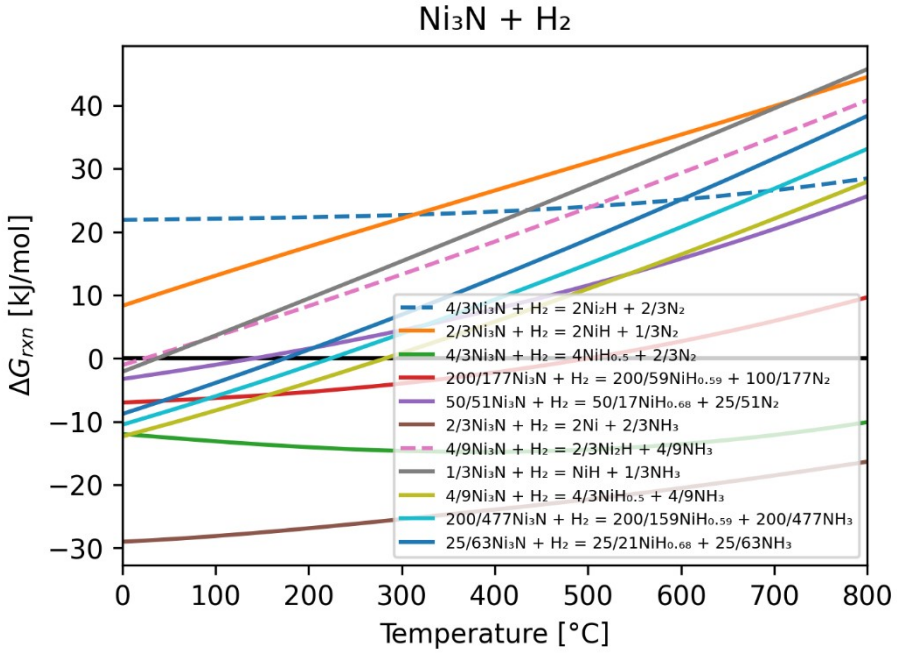

Figure S101: Ellingham diagram of the Ni_3N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

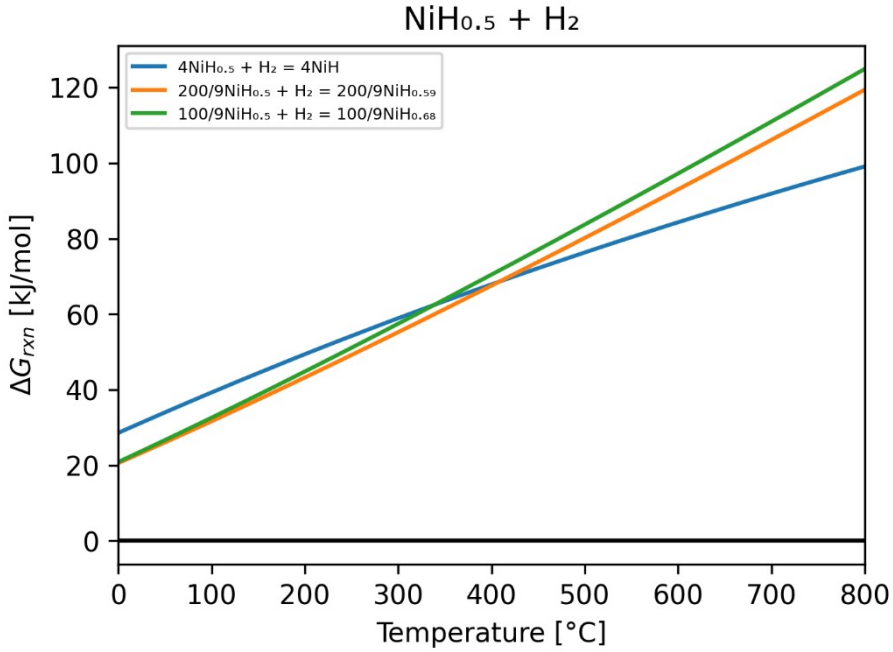

Figure S102: Ellingham diagram of the $NiH_{0.5}$ hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

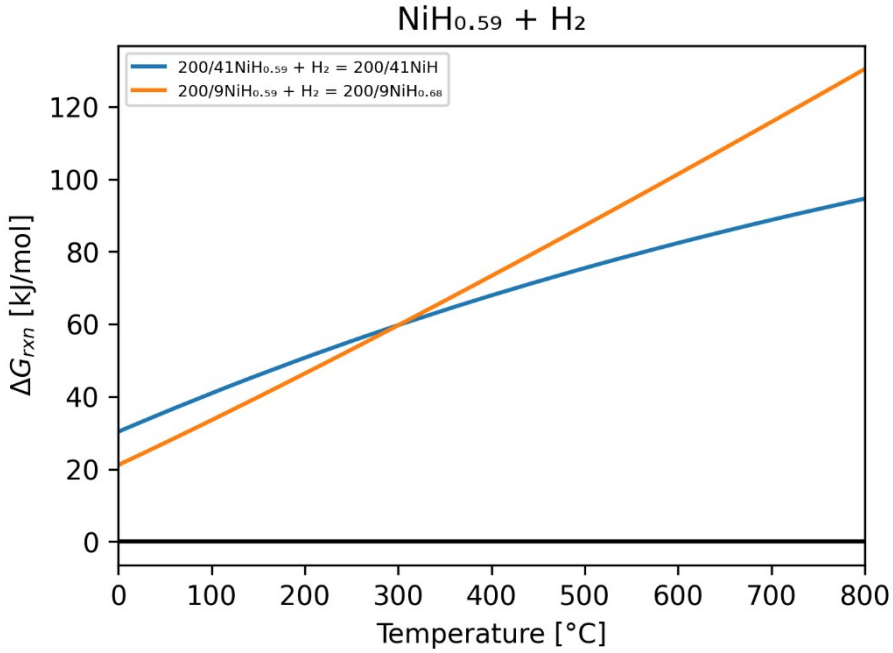

Figure S103: Ellingham diagram of the $NiH_{0.59}$ hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

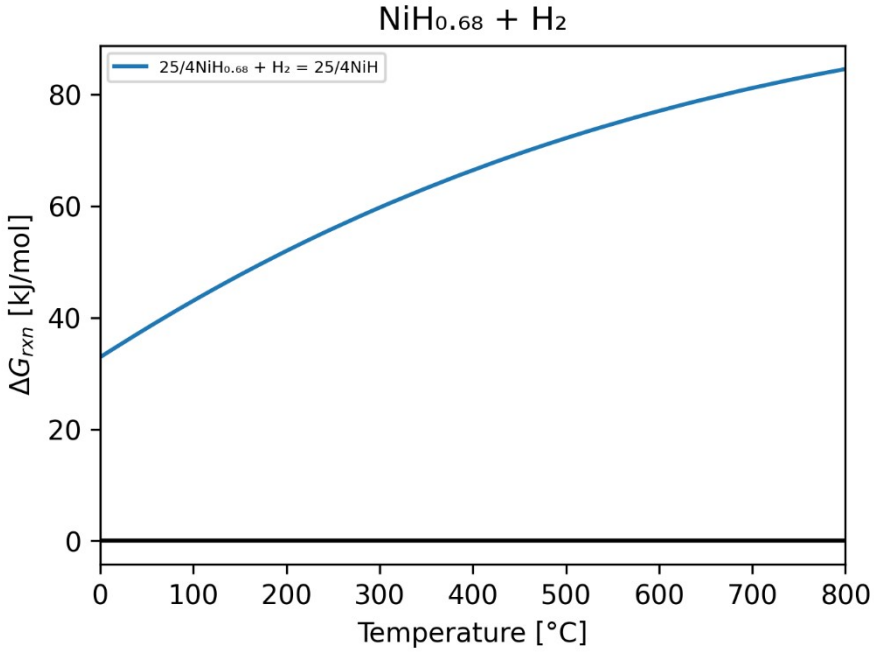

Figure S104: Ellingham diagram of the $NiH_{0.68}$ hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

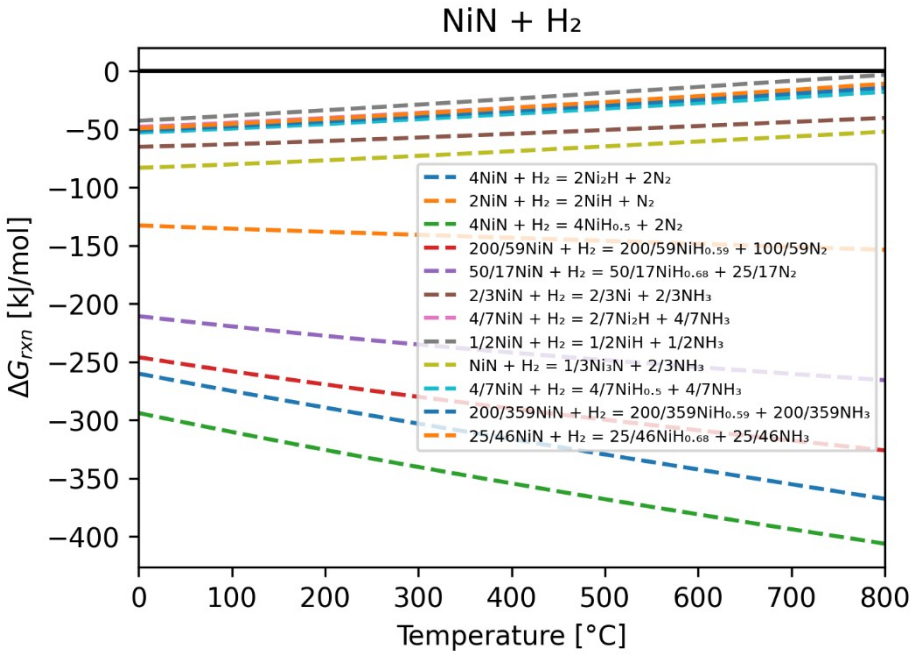

Figure S105: Ellingham diagram of the NiN hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

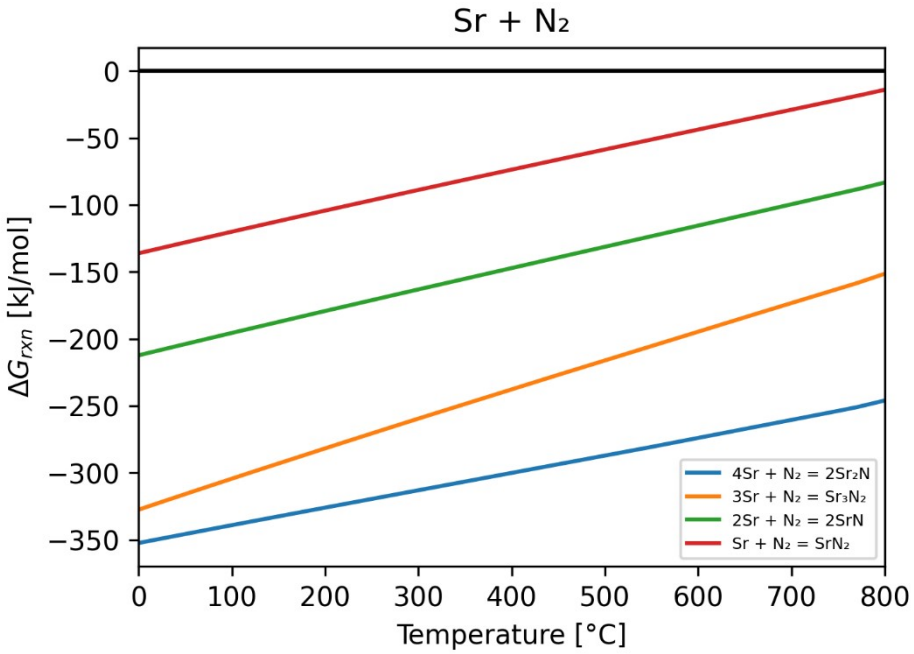

Figure S106: Ellingham diagram of the Sr nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

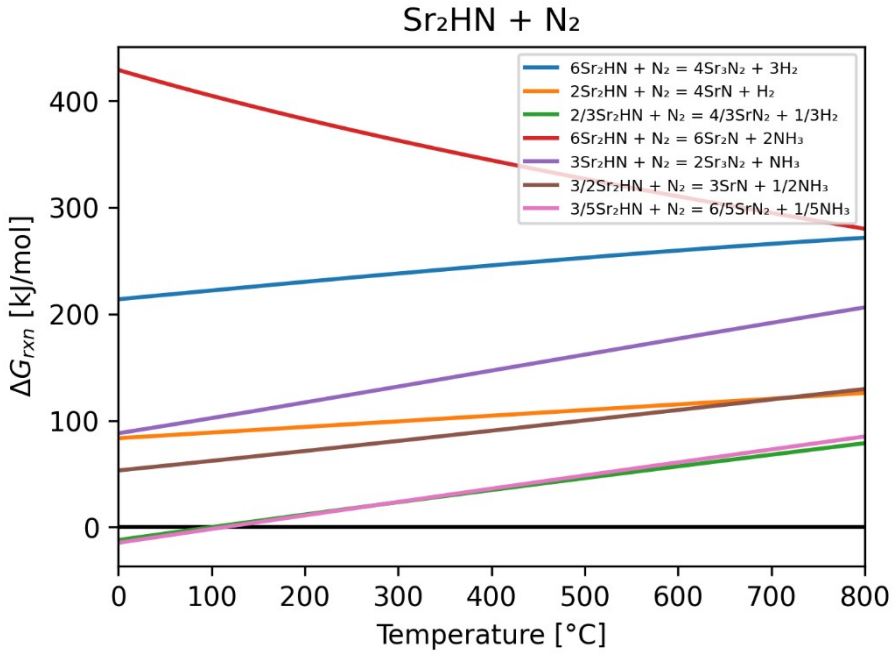

Figure S107: Ellingham diagram of the Sr_2HN nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

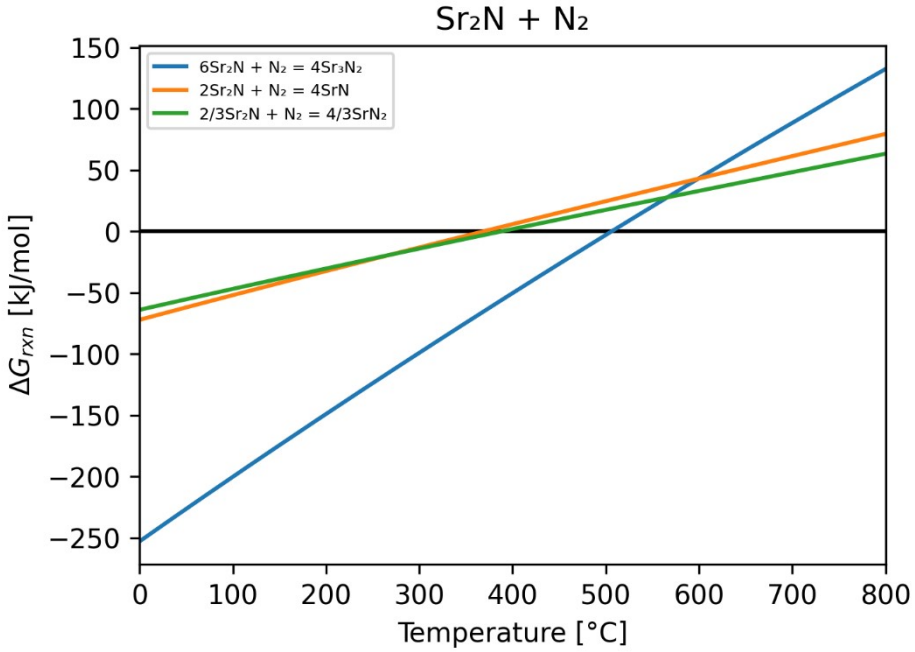

Figure S108: Ellingham diagram of the Sr_2N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

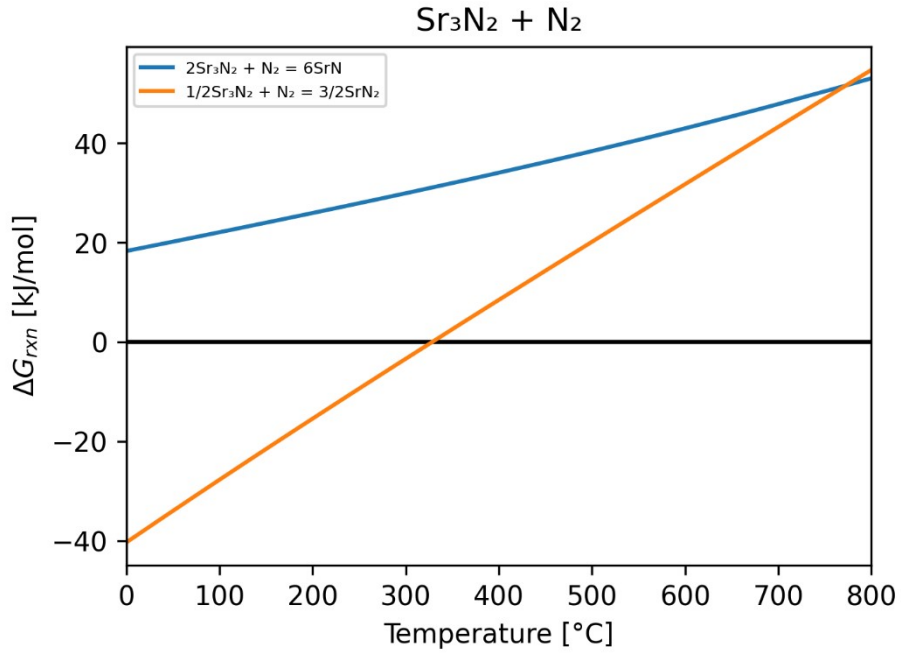

Figure S109: Ellingham diagram of the Sr_3N_2 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

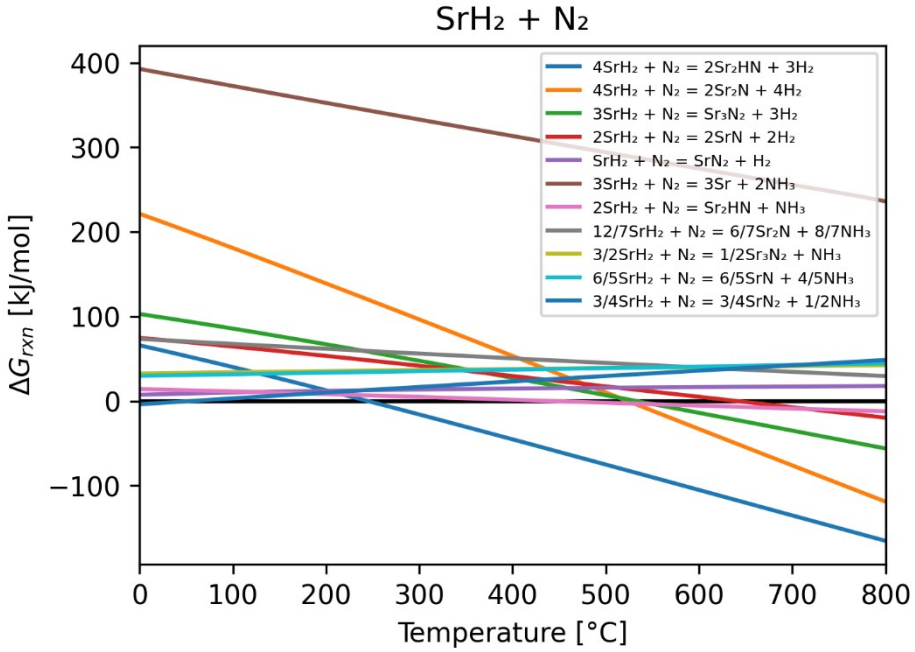

Figure S110: Ellingham diagram of the SrH_2 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

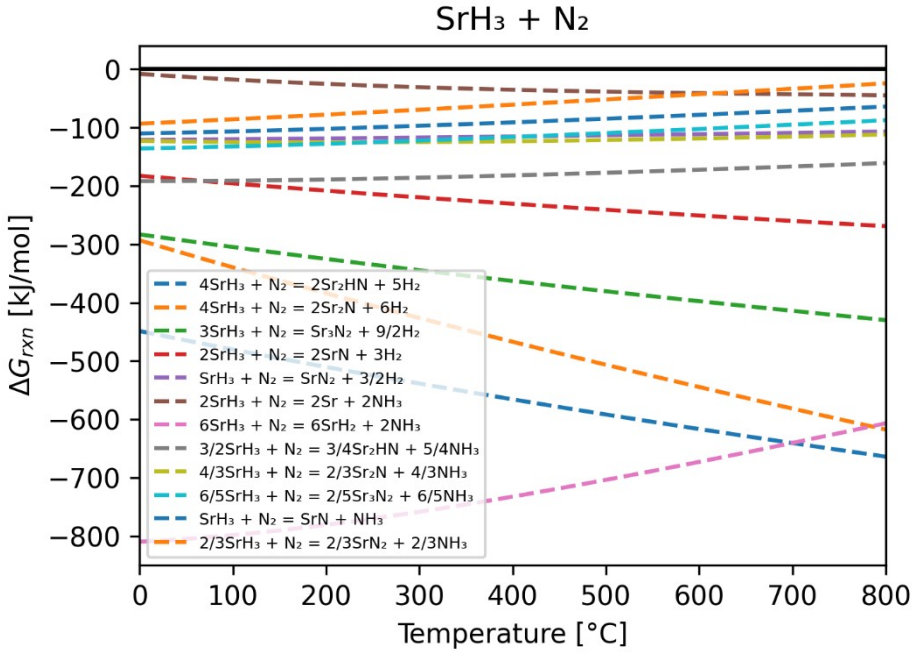

Figure S111: Ellingham diagram of the SrH_3 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

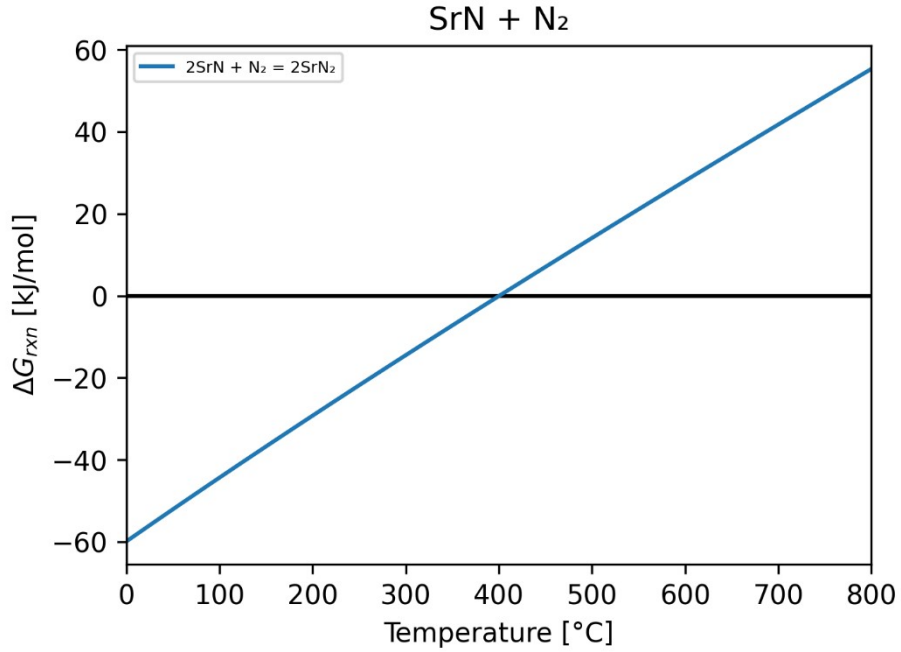

Figure S112: Ellingham diagram of the SrN nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

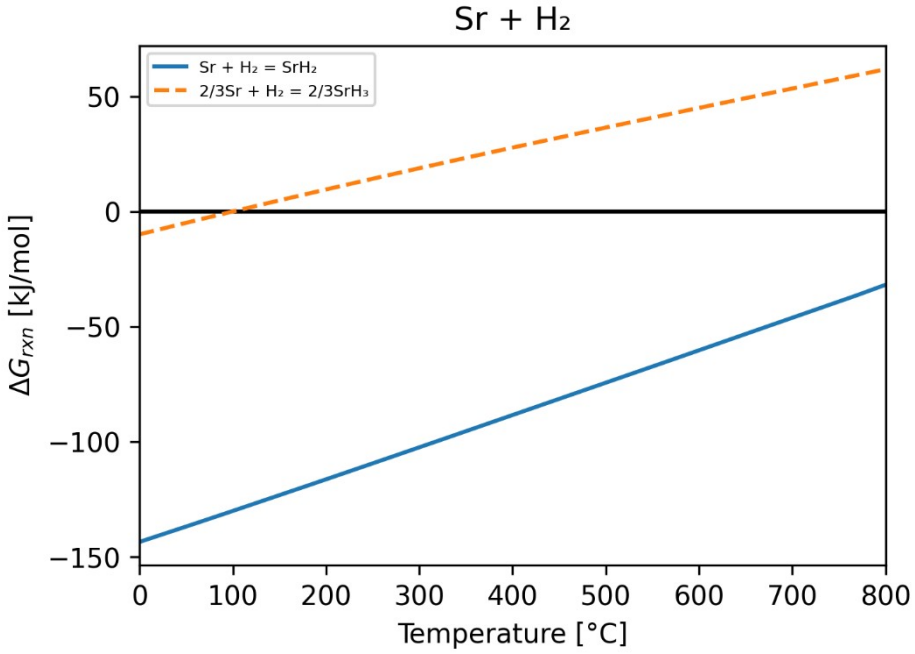

Figure S113: Ellingham diagram of the Sr hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

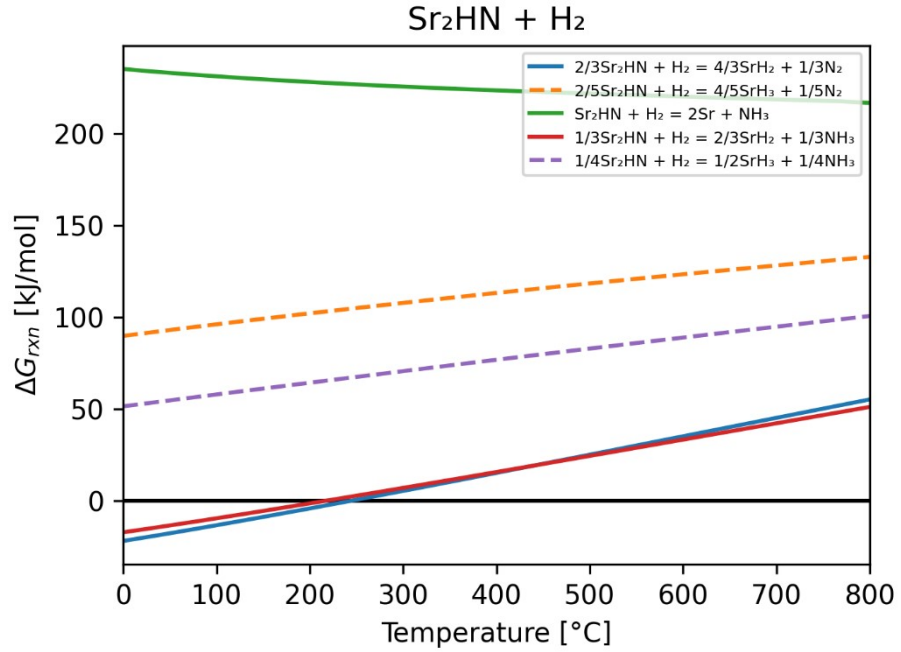

Figure S114: Ellingham diagram of the Sr_2HN hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

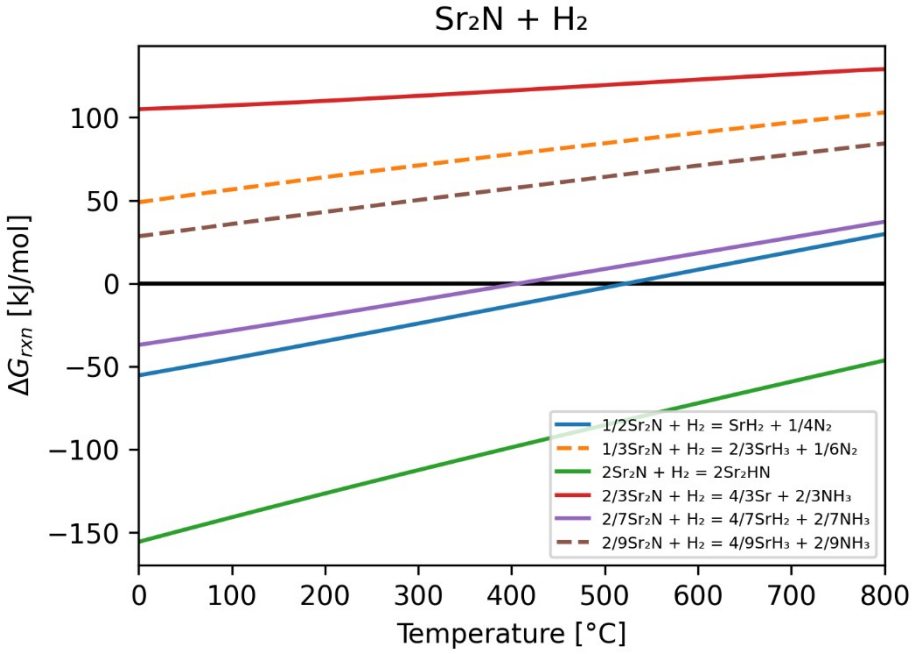

Figure S115: Ellingham diagram of the Sr_2N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

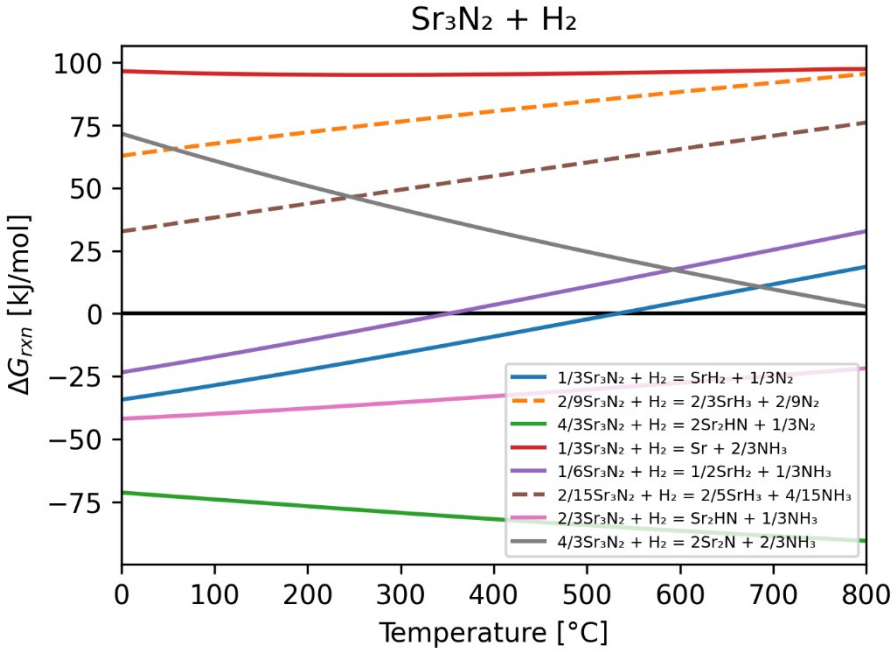

Figure S116: Ellingham diagram of the Sr_3N_2 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

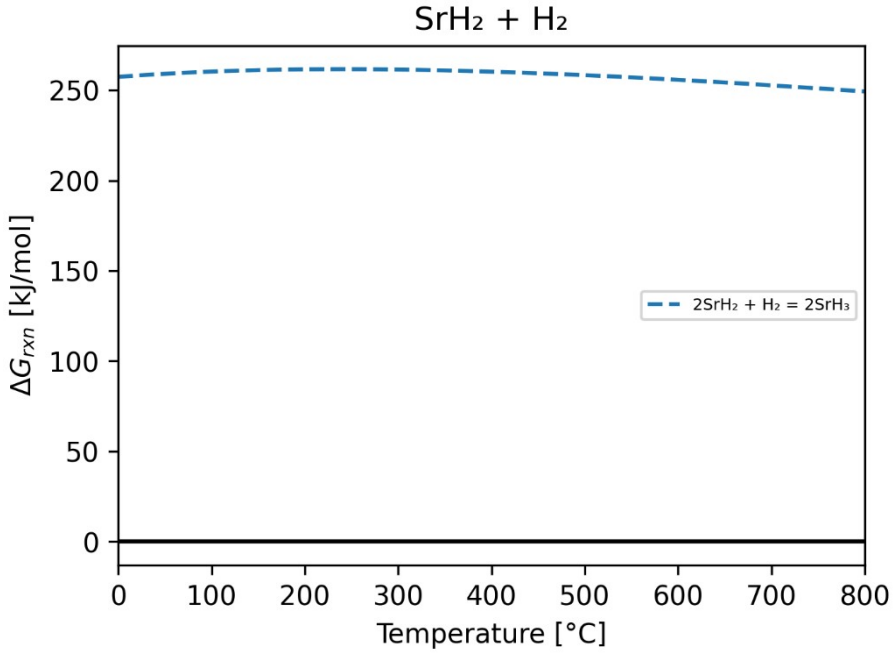

Figure S117: Ellingham diagram of the SrH_2 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

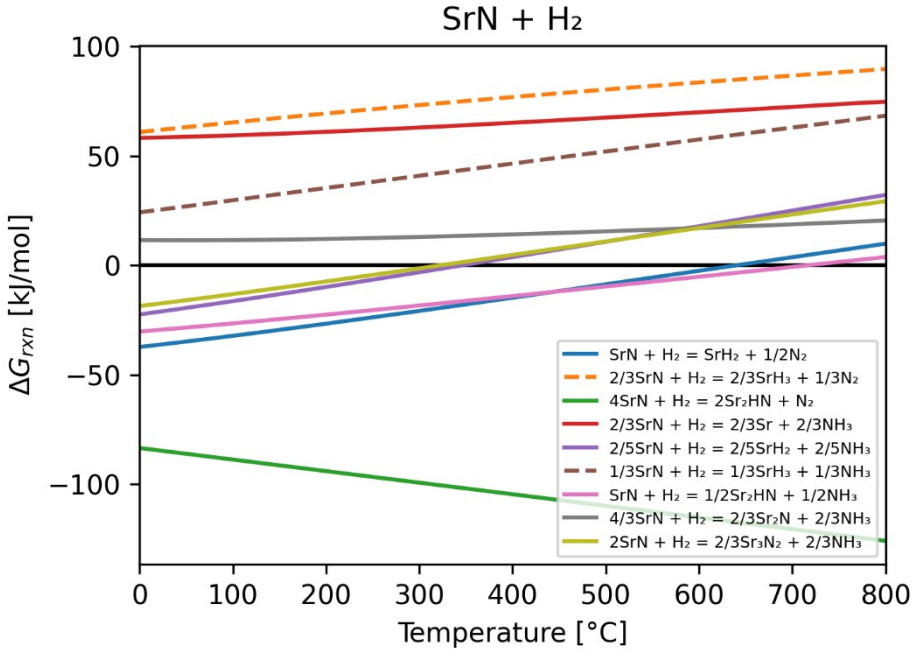

Figure S118: Ellingham diagram of the SrN hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

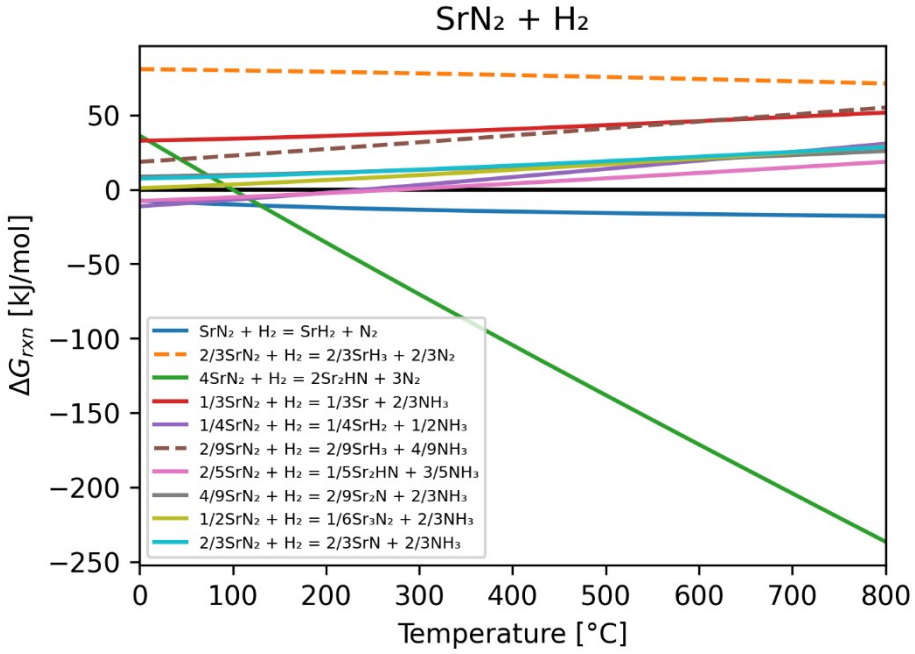

Figure S119: Ellingham diagram of the SrN_2 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

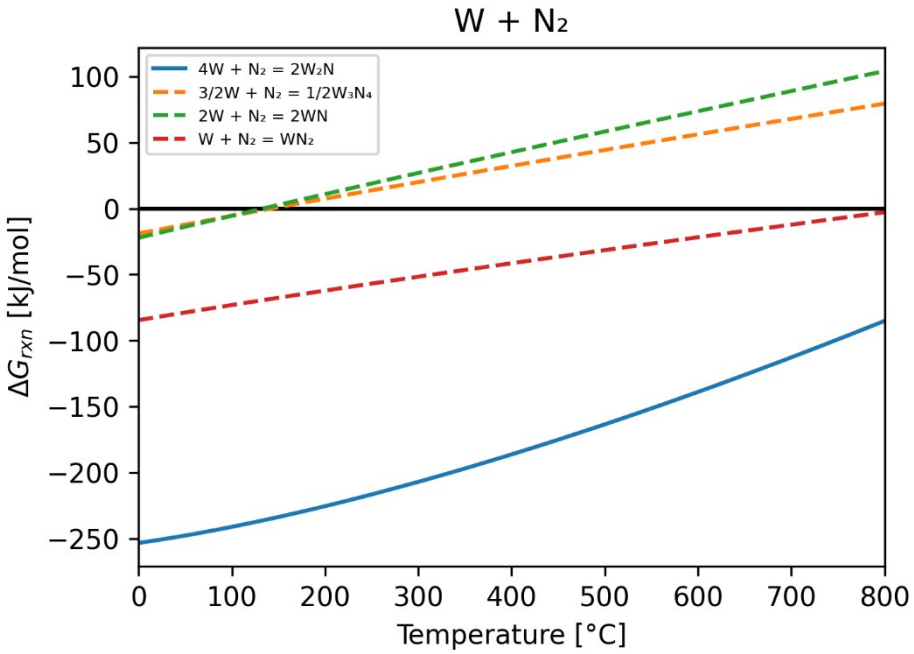

Figure S120: Ellingham diagram of the W nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

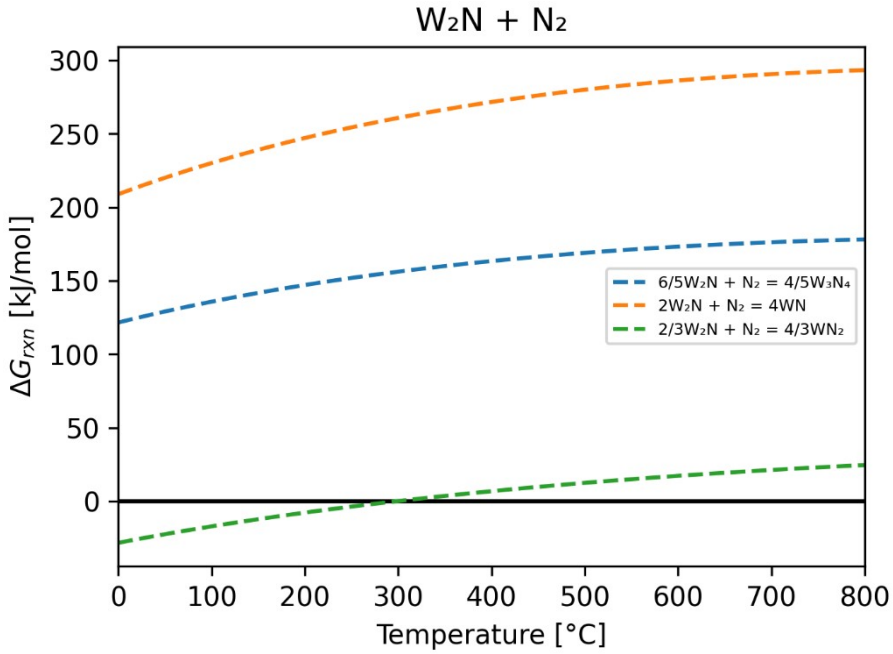

Figure S121: Ellingham diagram of the W_2N nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

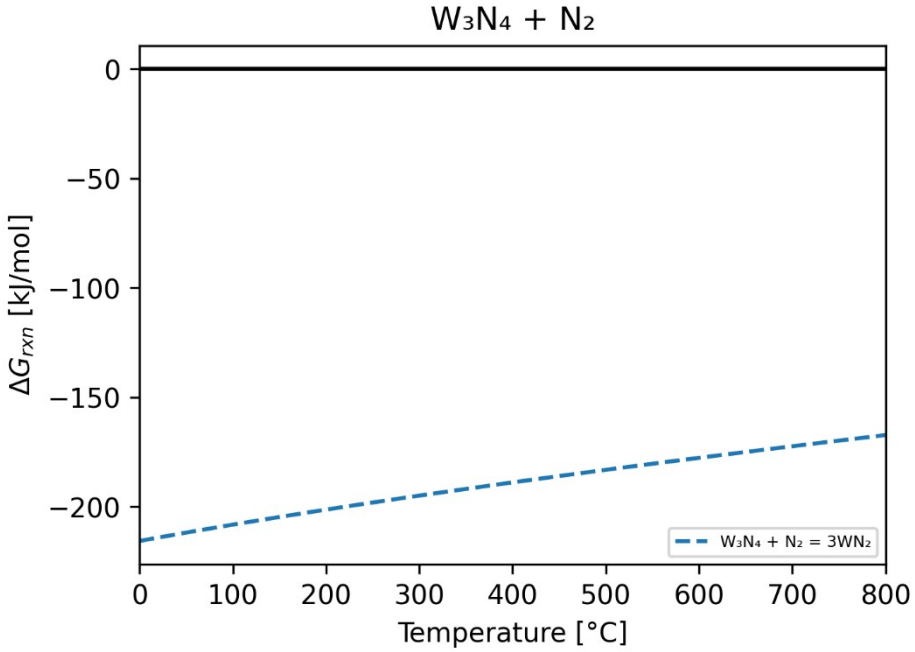

Figure S122: Ellingham diagram of the W_3N_4 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

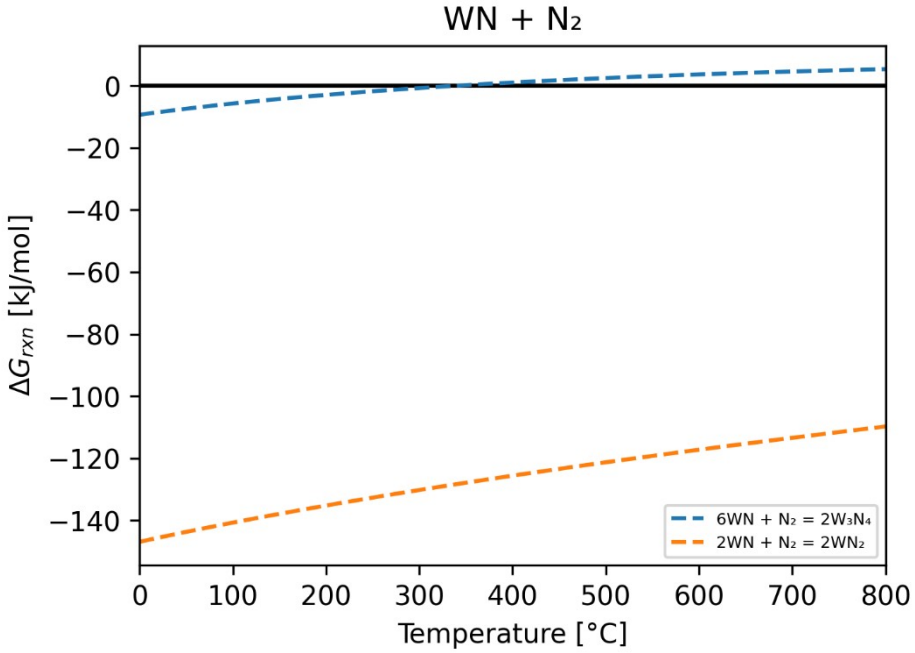

Figure S123: Ellingham diagram of the WN nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

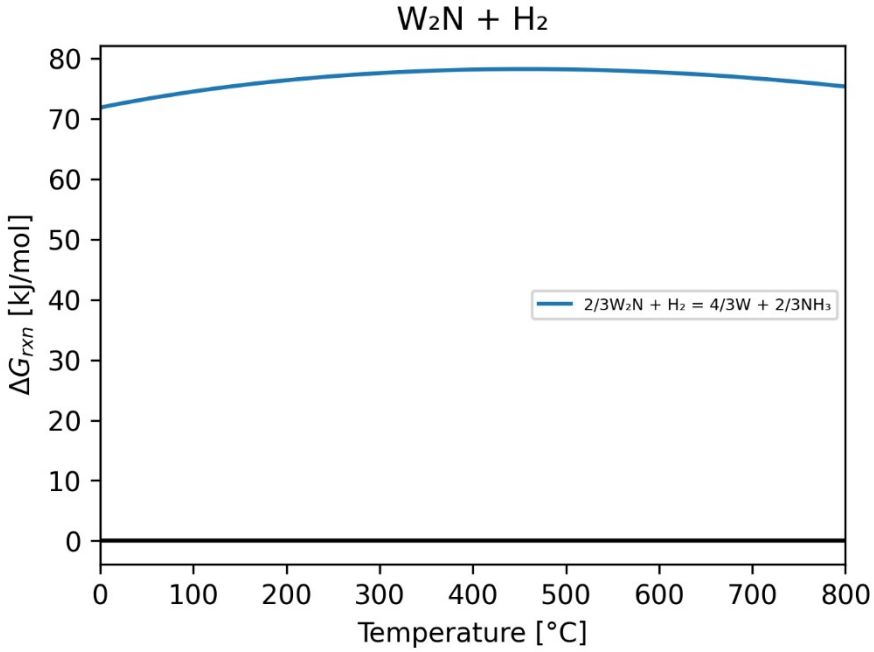

Figure S124: Ellingham diagram of the W_2N hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

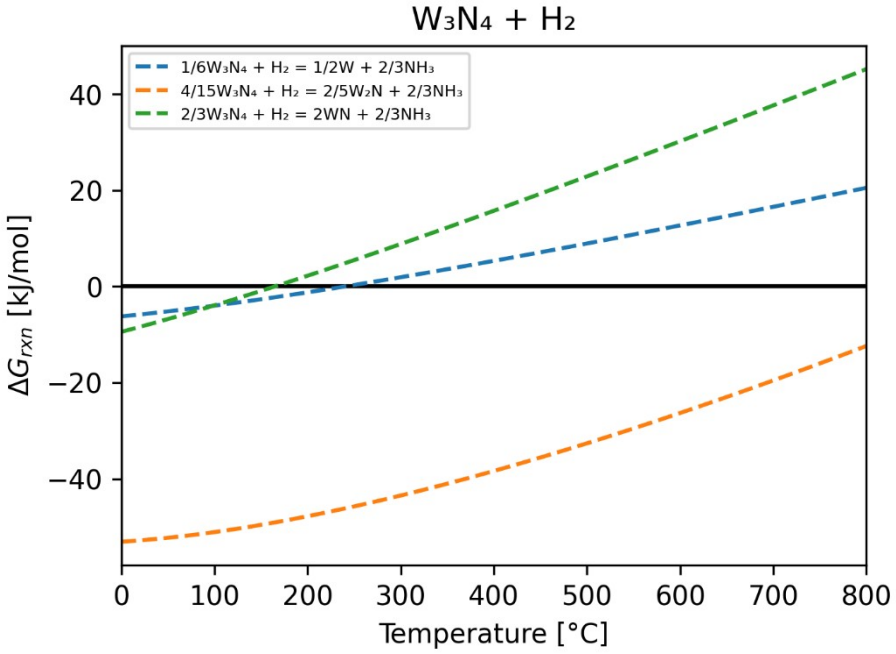

Figure S125: Ellingham diagram of the W_3N_4 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

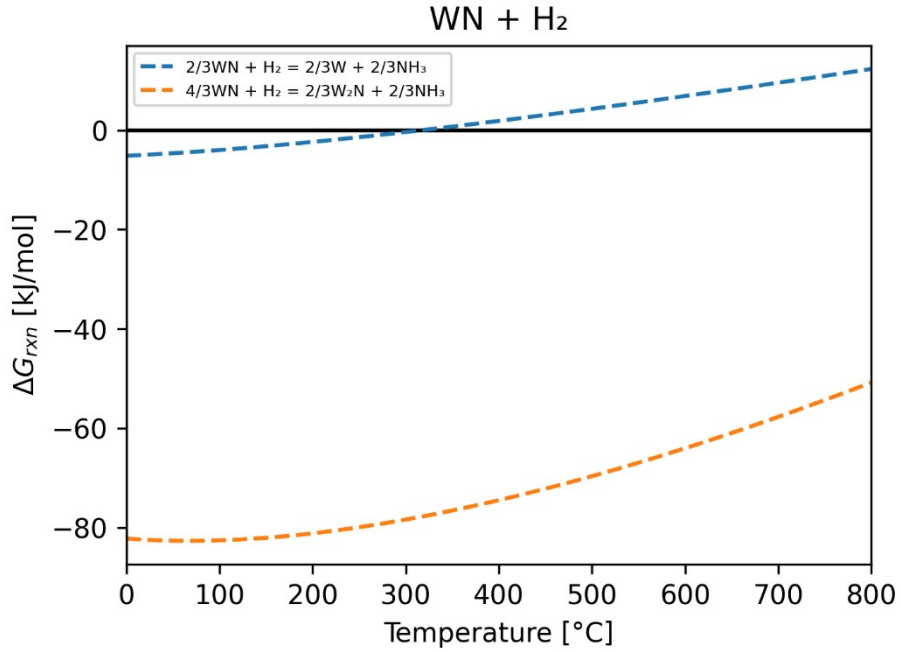

Figure S126: Ellingham diagram of the WN hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

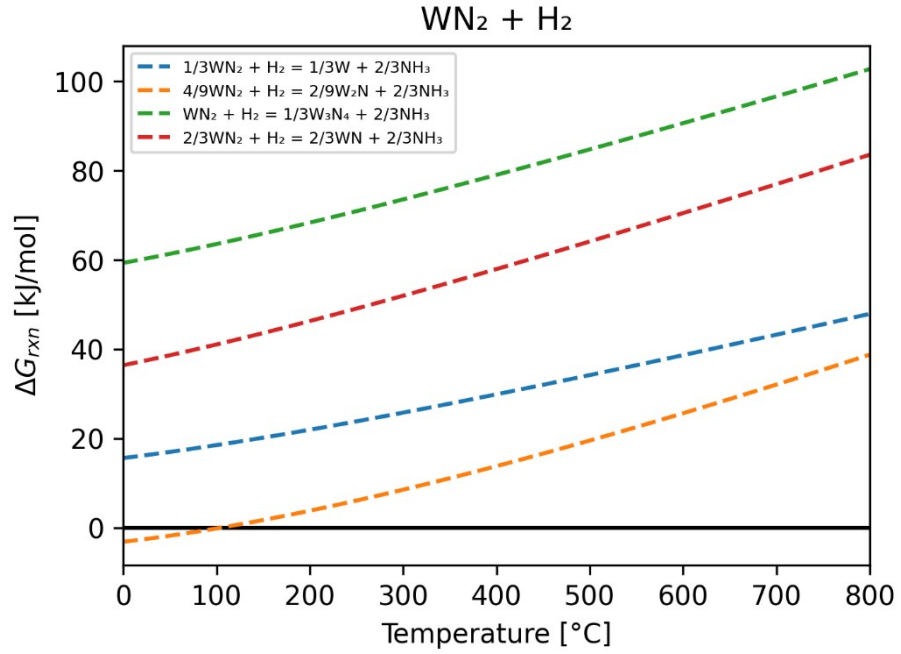

Figure S127: Ellingham diagram of the WN_2 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

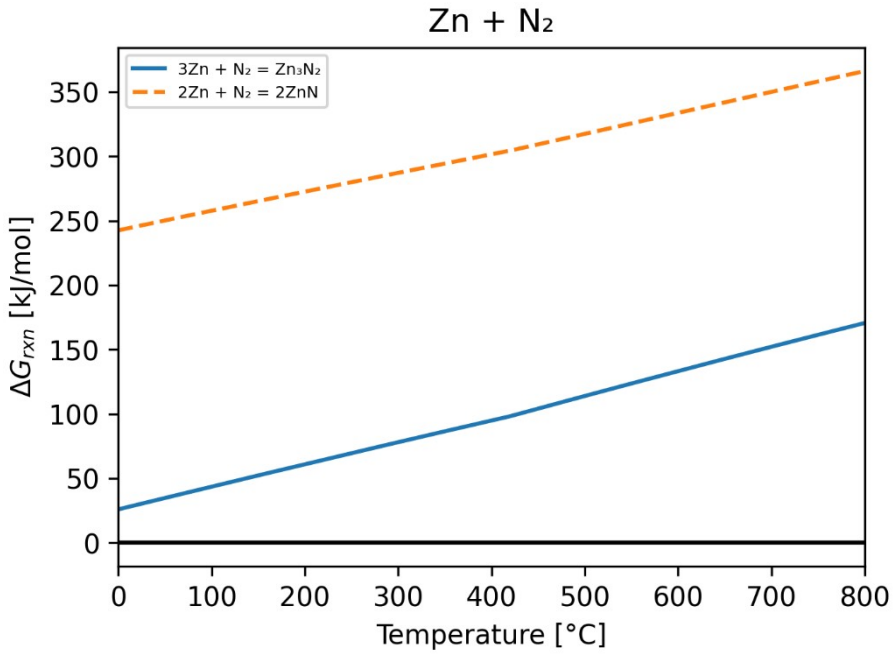

Figure S128: Ellingham diagram of the Zn nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

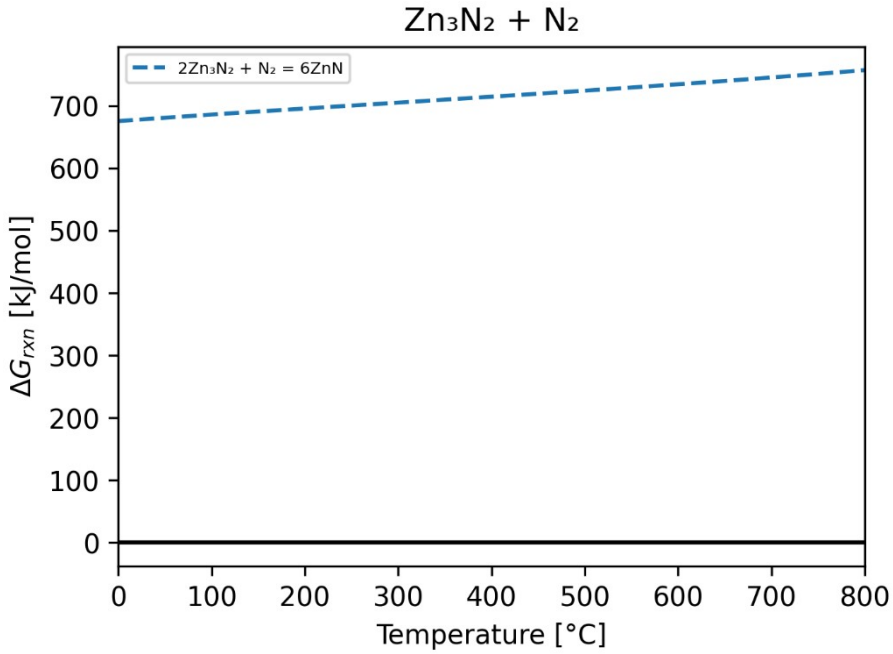

Figure S129: Ellingham diagram of the Zn_3N_2 nitridation step: standard Gibbs free energy change per mol N_2 as a function of temperature.

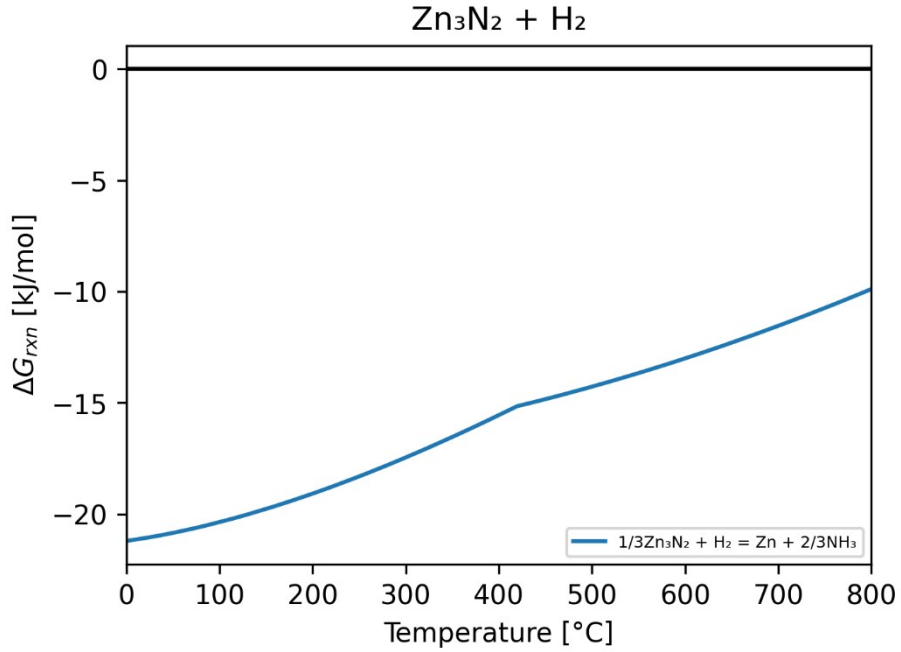

Figure S130: Ellingham diagram of the Zn_3N_2 hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

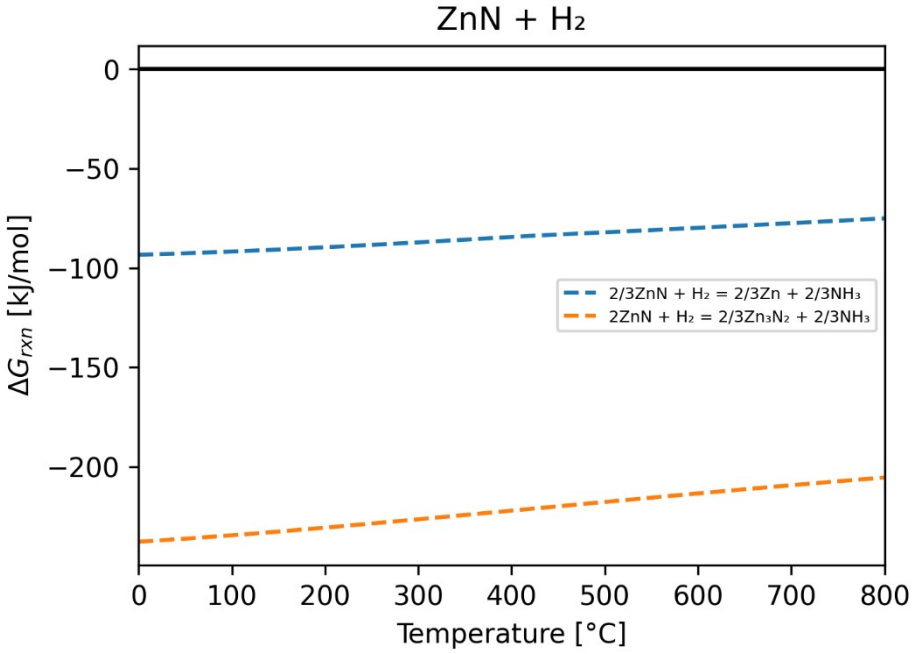

Figure S131: Ellingham diagram of the ZnN hydrogenation step: standard Gibbs free energy change per mol H_2 as a function of temperature.

2. Experimental Screening

Experimental screening was performed by thermogravimetric runs. The plots show the variation of mass and temperature (recorded by the TGA), ion current (recorded by the mass spectrometer), and were applicable the NH_3 concentration (recorded by the NH_3 analyzer) as a function of time. The materials used in the experiments are shown in Table S29.

Table S29: List of materials used in TGA experiments.

Material	Form	Size	Purity [%]	Supplier
Sr	Random pieces	Flakes in mm-range size	99	Sigma-Aldrich (Merck)
Sr	Granules	mm-range size	99	Sigma-Aldrich (Merck)
Mn	Powder	-325 mesh	99.3	Alfa Aesar
Ca	Granules	-16 mesh	99.5	Alfa Aesar
Cr	Powder	APS <10 micron	99.2	Alfa Aesar
Cu	Powder	-625 mesh	99	Alfa Aesar
W	Powder	APS 1-5 micron	99.9	Alfa Aesar
Ni	Powder	APS 3-7 micron	99.9	Alfa Aesar
Mo	Powder	APS 2-4 micron	99.9	Alfa Aesar
Fe	Powder	APS <10 micron	99.9+	Alfa Aesar
Zn	Powder	Average 4-7 micron	97.5	Alfa Aesar
Co	Powder	APS 1.6 micron	99.8	Alfa Aesar
Al	Powder	APS 3 micron	99.9	Nanografi Nano Technology
Li	Granules	4-10 mesh	99	Sigma-Aldrich (Merck)

The Al-based system

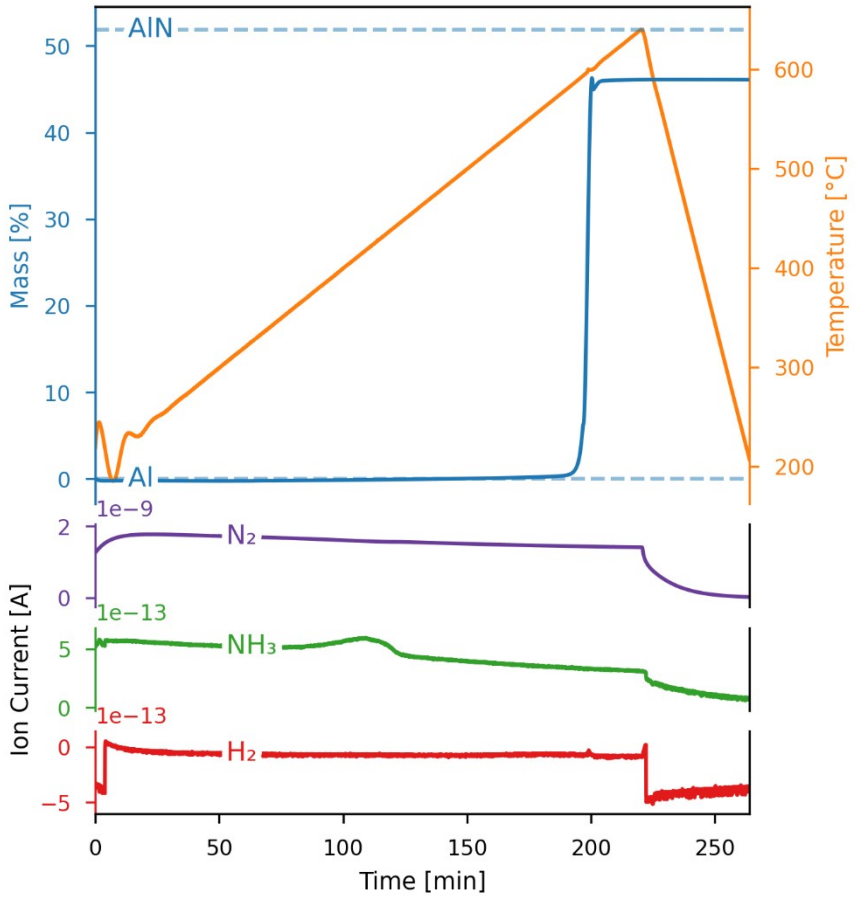

Figure S132: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Al-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%) and full conversion to AlN (51.91%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 200-640°C at a rate of 2°C/min in 100% N_2 and cooled down back to 200°C in 100% Ar. Al reacted to AlN, in agreement with the Ellingham diagram (

Table S1).

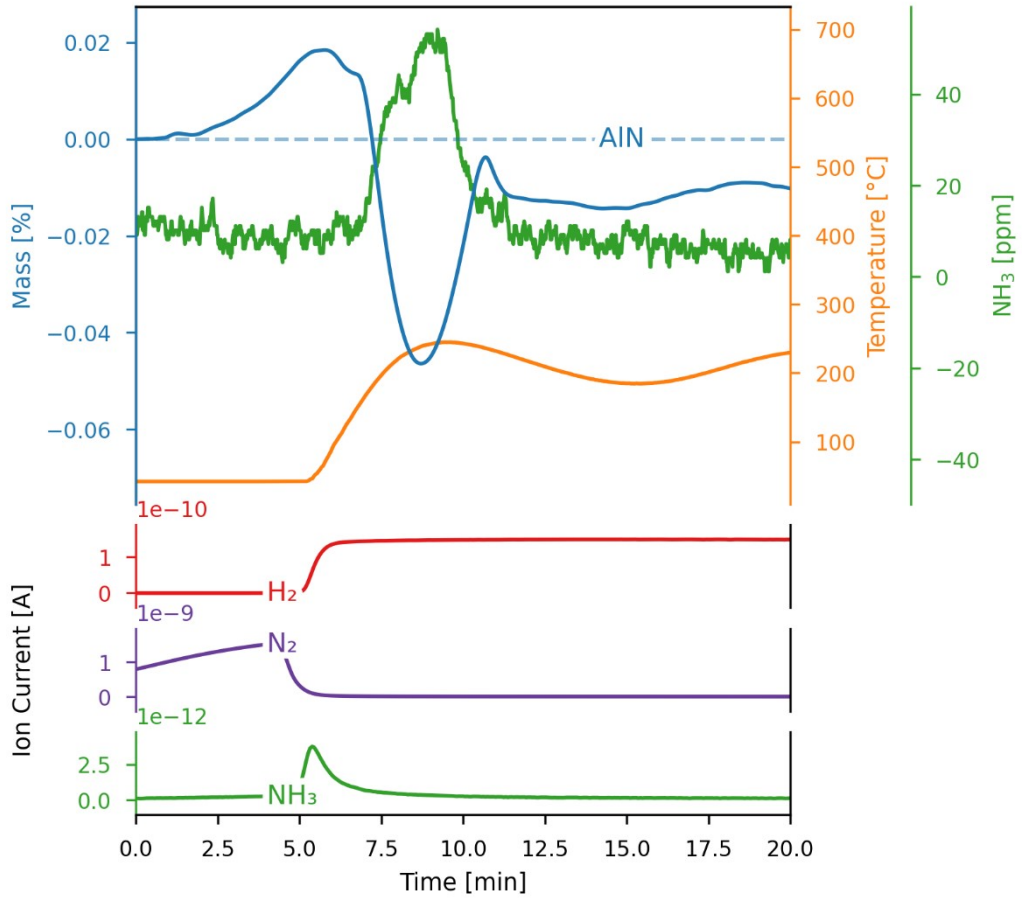

Figure S133: Variations of mass and temperature (recorded by the TGA), ion current (recorded by the mass spectrometer), and NH_3 concentration (recorded by the NH_3 analyzer) as a function of time for the AlN-hydrogenation under 5% H_2 in Ar. Blue dashed line: theoretical mass changes for no conversion (0%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 200-700°C at a rate of 2°C/min in 5% H_2 in Ar (shown is a cropped version of the run to focus on the part with NH_3 production). Upon switching from a 100% N_2 flow to the 5% H_2 flow at around 10 minutes, the NH_3 analyzer registers a peak of NH_3 (approximately 40 ppm in the unfiltered signal).

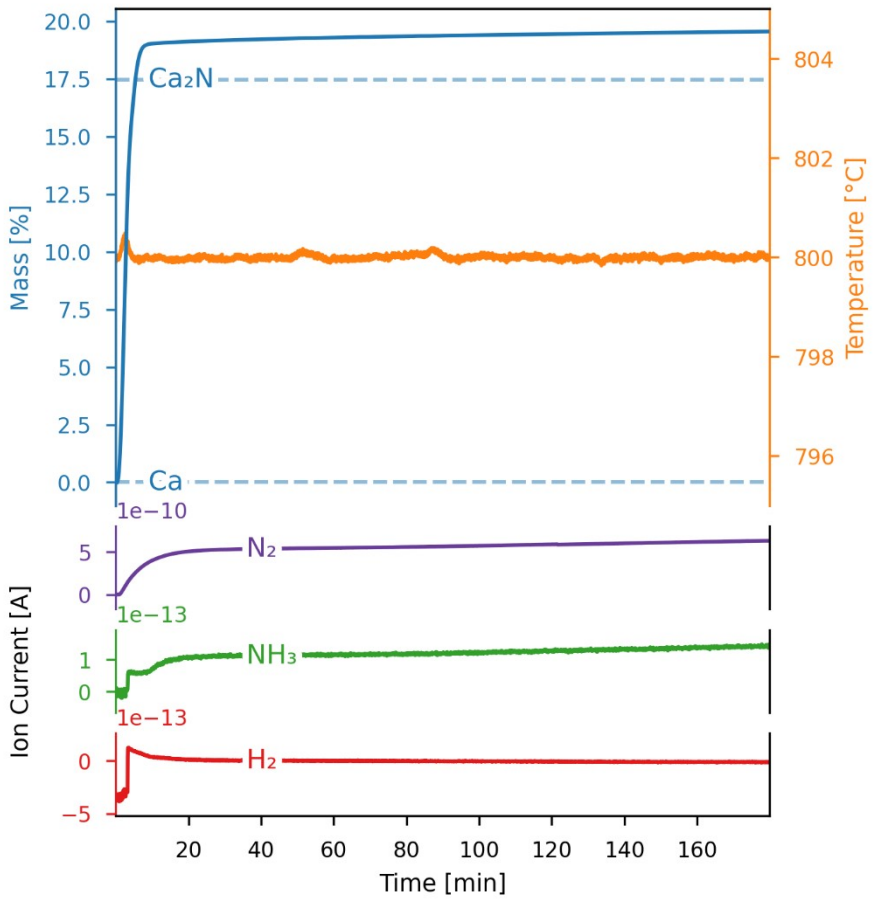

Figure S134: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Ca-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%) and full conversion to Ca_2N (17.47%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated to 800°C in Ar, then switched to 100% N_2. Ca reacted to Ca_2N, in agreement with the Ellingham diagram (Figure S6).

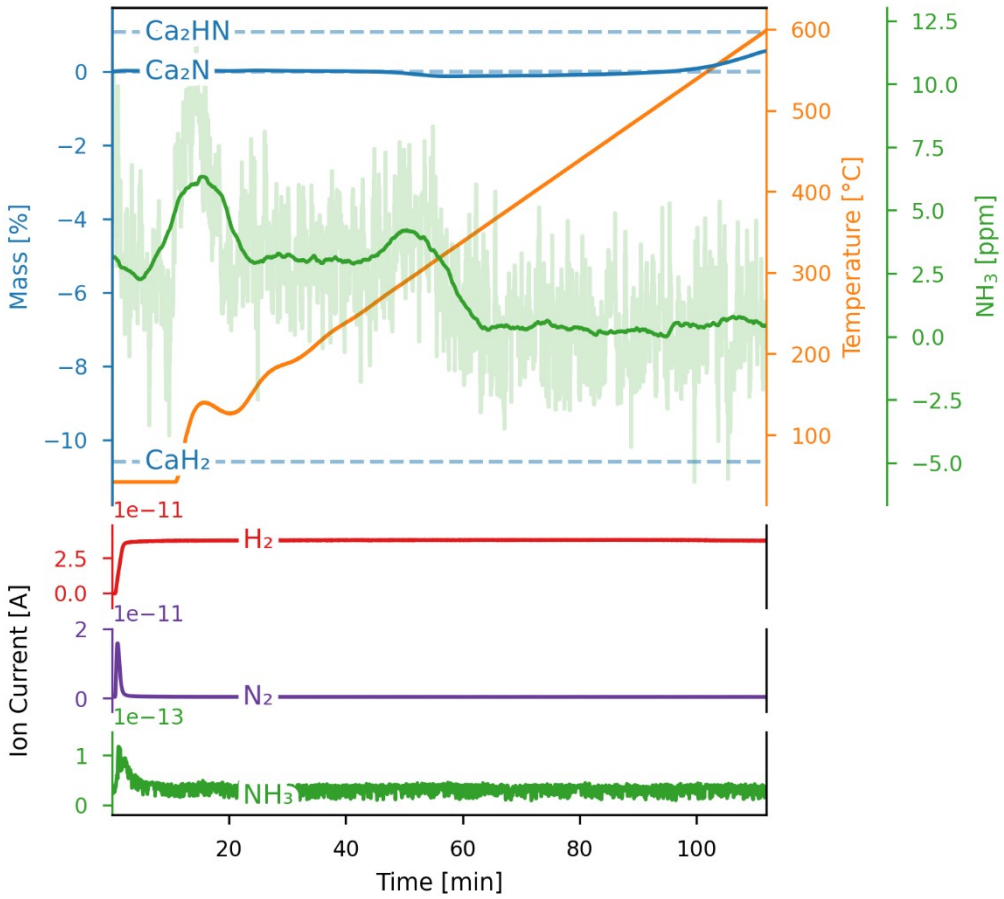

Figure S135: Variations of mass and temperature (recorded by the TGA), ion current (recorded by the mass spectrometer), and NH_3 concentration (recorded by the NH_3 analyzer) as a function of time for the Ca_2N -hydrogenation under 5% H_2 in Ar. Blue dashed line: theoretical mass changes for no conversion (0%), full conversion to CaH_2 (-10.59%), and full conversion to Ca_2HN (1.67%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Two peaks of NH_3 are visible in the filtered NH_3 signal, albeit very small (same order magnitude as the noise). The first peak is not accompanied by a change in the mass signal. The second peak, shortly before 300°C, is accompanied by a minor decrease in mass. According to the Ellingham diagram in Figure S12, the formation of CaH_2 with either N_2 or NH_3 from the hydrogenation of Ca_2N is spontaneous up to approximately that temperature.

The Co-based system

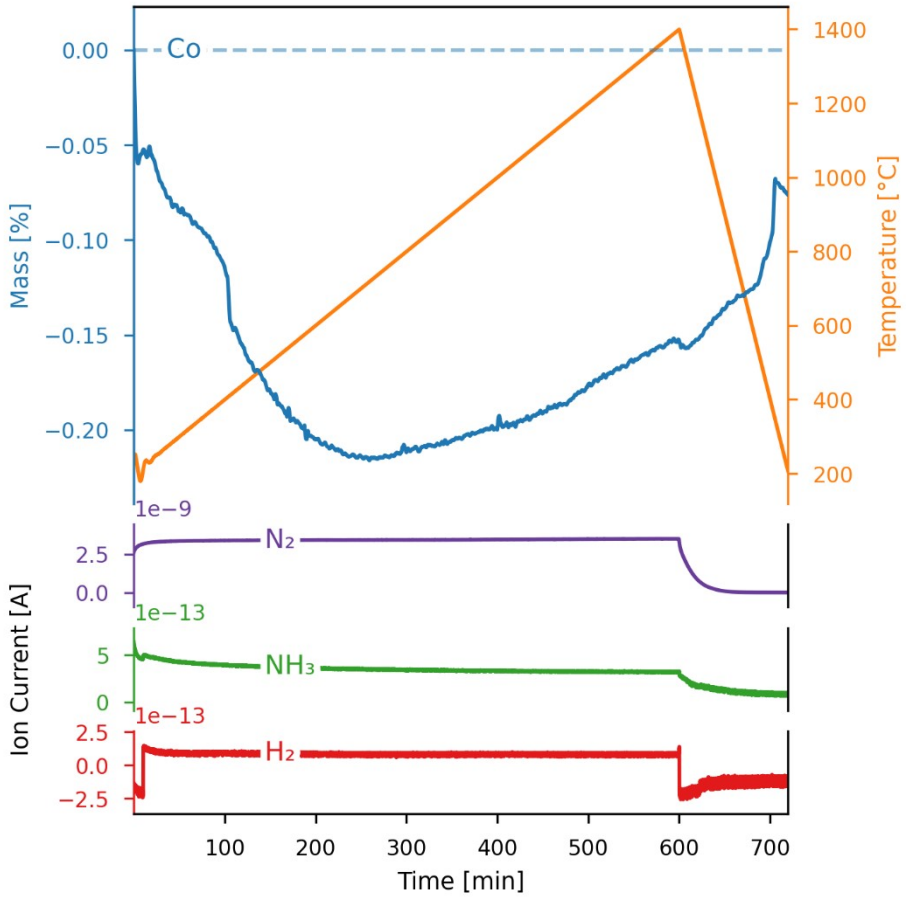

Figure S136: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Co-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 200-1400°C at a rate of 2°C/min in 100% N_2 and cooled down back to 200°C in 100% Ar. No significant reaction was measurable, in agreement with the Ellingham diagram (Figure S16).

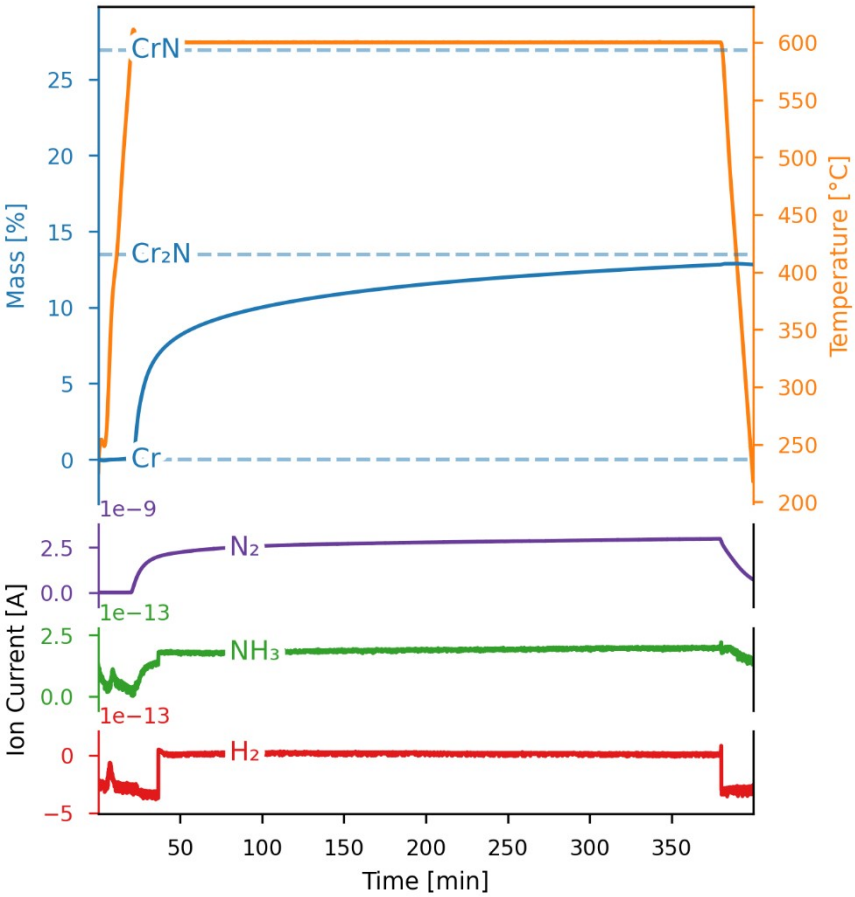

Figure S137: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Cr-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%), full conversion to Cr_2N (13.47%), and full conversion to CrN (26.94%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated to 600°C in Ar, then switch to 100% N_2. Cr reacted to Cr_2N, in agreement with the Ellingham diagram (Figure S24).

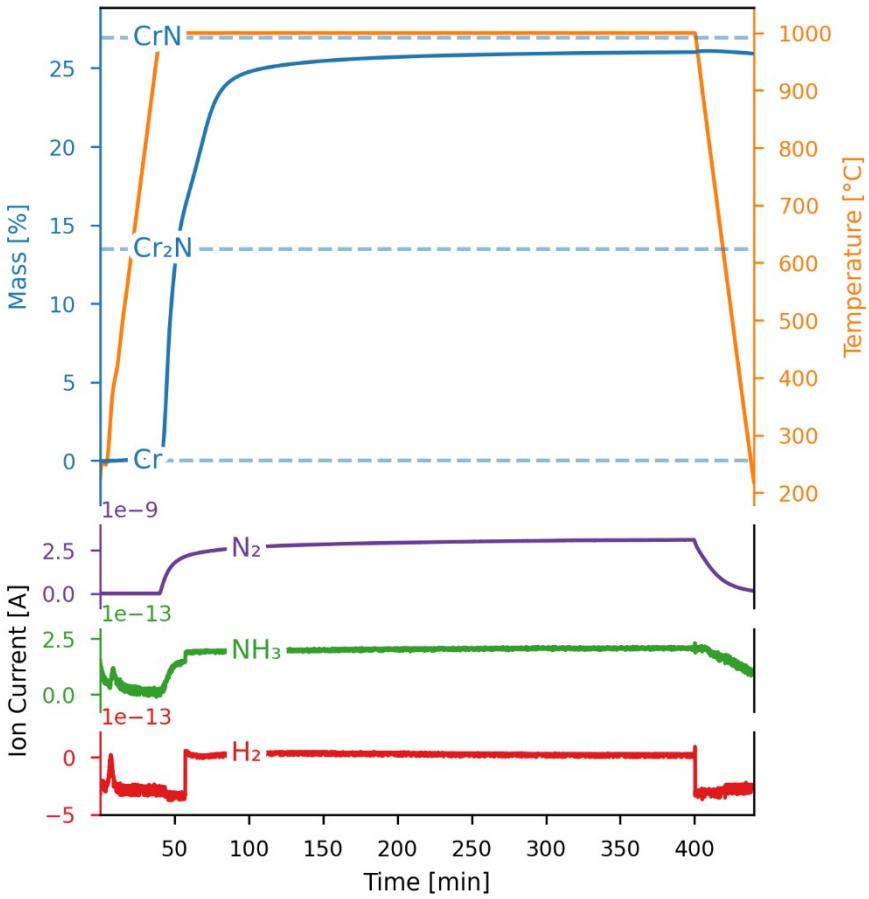

Figure S138: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Cr-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%), full conversion to Cr_2N (13.47%), and full conversion to CrN (26.94%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated to 600°C in Ar, then switch to 100% N_2. Cr reacted to CrN. According to the Ellingham diagram (Figure S24), the formation of Cr2N should be more favourable in this temperature range.

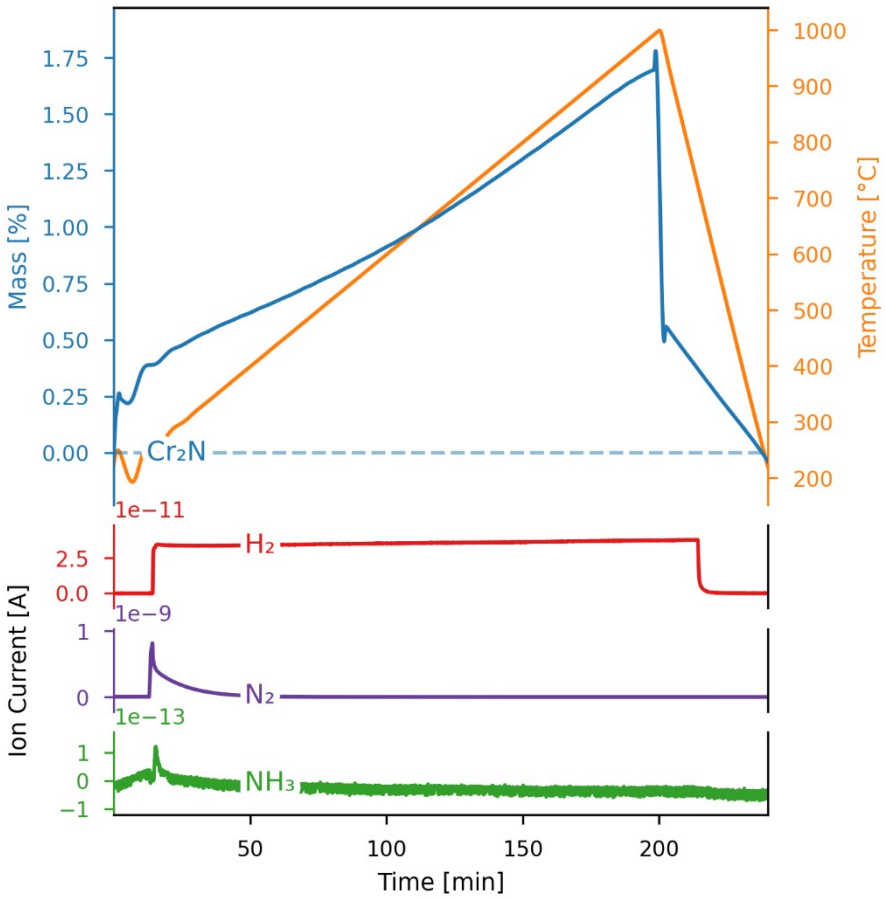

Figure 139: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Cr_2N-hydrogenation under 5% H. in Ar. Blue dashed lines: theoretical mass changes for no conversion (0%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 200-1000°C at a rate of 4°C/min in 5% H_2 in Ar and cooled down back to 200°C in 100% Ar. No significant reaction was measurable, in agreement with the Ellingham diagram (Figure S31).

The Cu-based system

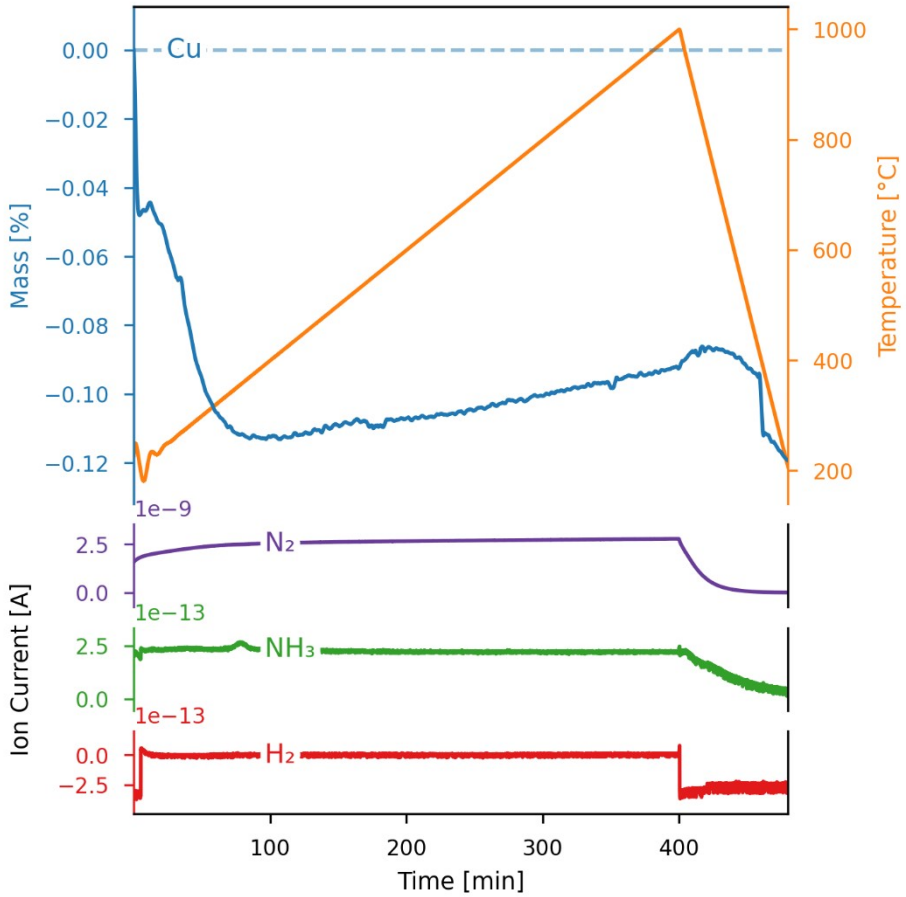

Figure S140: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Cu-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 200-1000°C at a rate of 2°C/min in 100% N_2 and cooled down back to 200°C in 100% Ar. No significant reaction was measurable, in agreement with the Ellingham diagram (Figure S36).

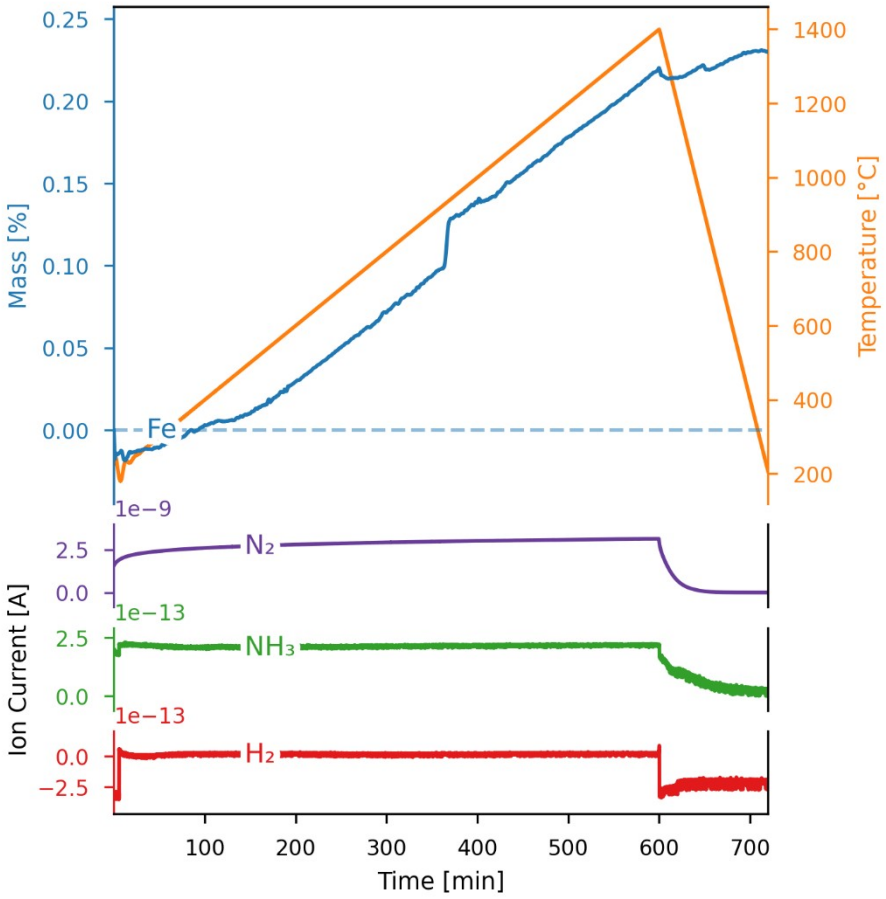

Figure S141: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Fe-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 200-1400°C at a rate of 2°C/min in 100% N_2 and cooled down back to 200°C in 100% Ar. No significant reaction was measurable. According to the Ellingham diagram (Figure S46), the formation of Fe_3N and FeN should be favourable up to 220°C and 450°C, respectively.

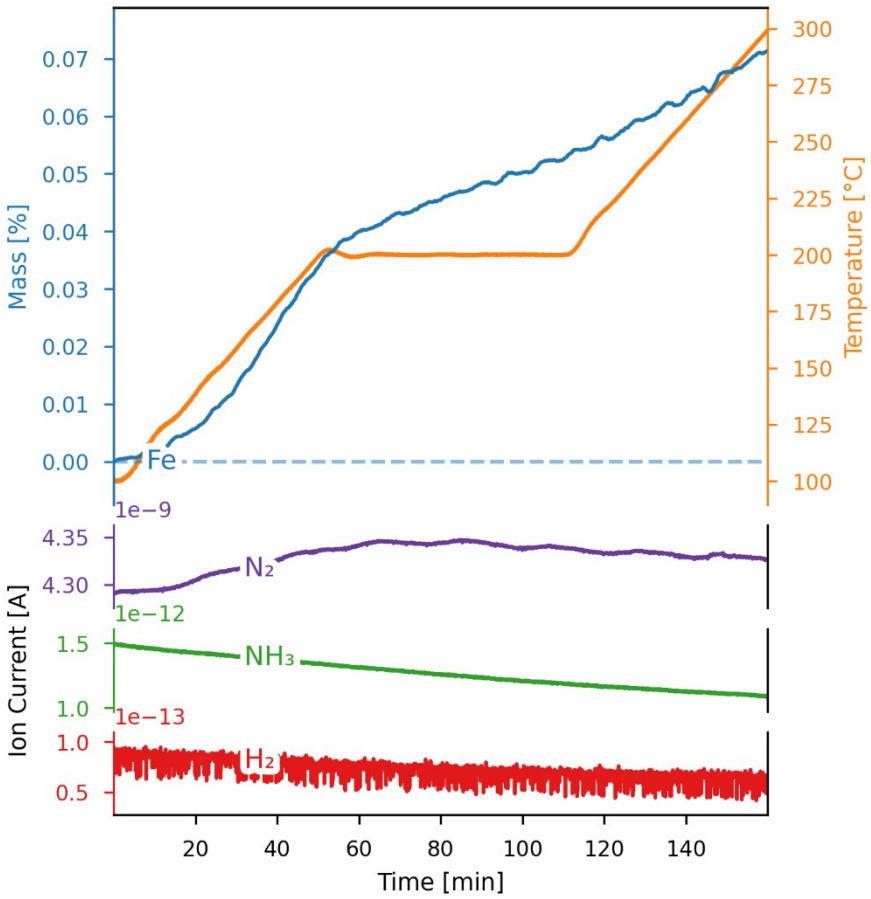

Figure S142: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Fe-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 100-300°C at a rate of 2°C/min in 100% N_2 with an isothermal section of 60 min at 200°C in between. No significant reaction was measurable. According to the Ellingham diagram (Figure S46), the formation of Fe_3N and FeN should be favourable up to 220°C and 450°C, respectively.

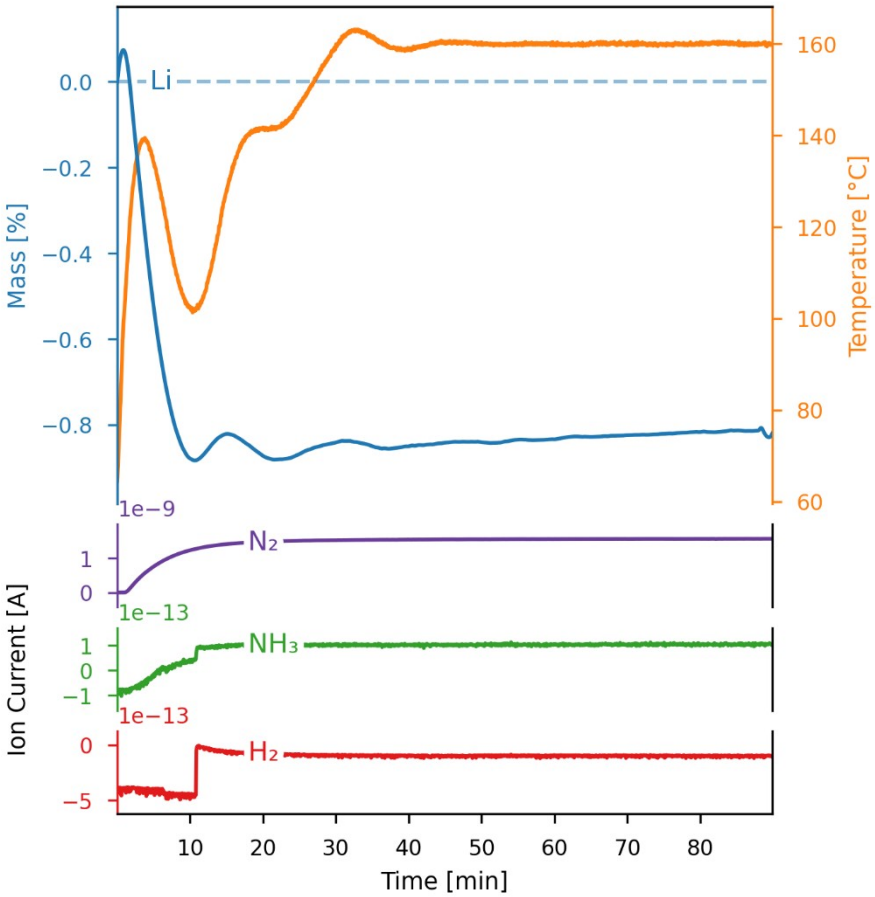

Figure S143: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Li-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated to 160°C in Ar, then switched to 100% N_2. No significant reaction was measurable. According to the Ellingham diagram (Figure S62), the formation of Li_3N should be favourable at that temperature. The low temperature seems to prevent the reaction from proceeding. Due to the Li melting point of 180.5°C at 1 bar, higher temperatures are not feasible.

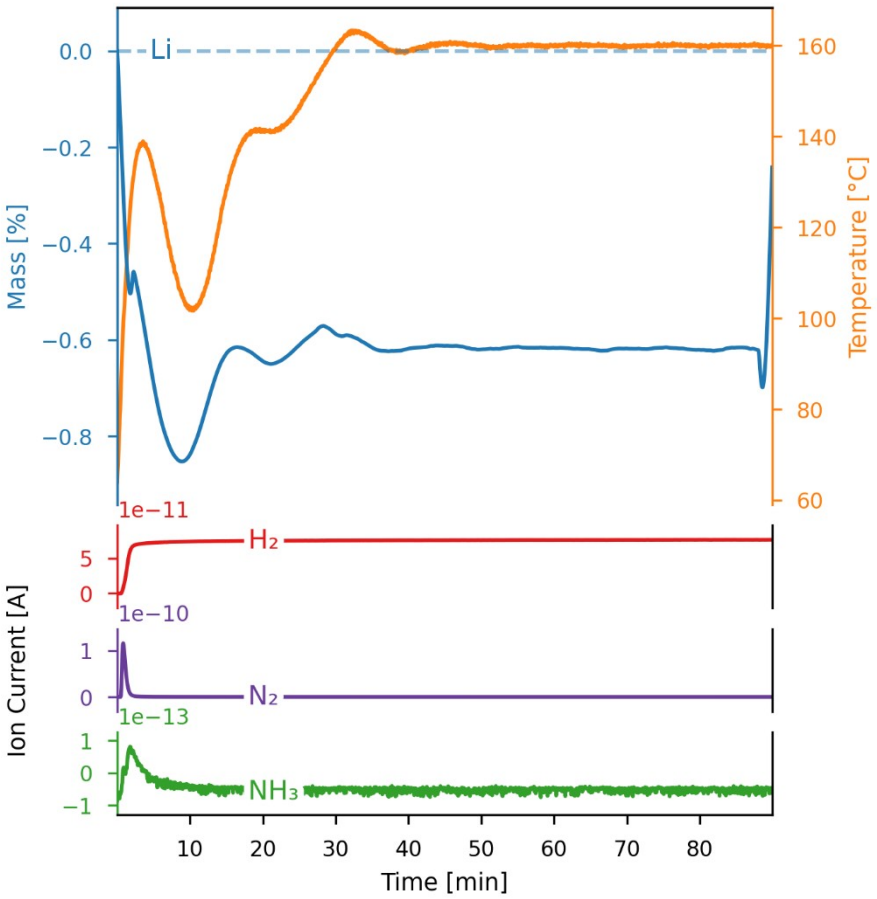

Figure S144: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Li-hydrogenation under 5% H_2 in Ar. Blue dashed lines: theoretical mass changes for no conversion (0%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated to 160°C in Ar, then switched to 5% H_2 in Ar. No significant reaction was measurable. According to the Ellingham diagram (Figure S66), the formation of LiH should be favourable at that temperature. The low temperature seems to prevent the reaction from proceeding. Due to the Li melting point of 180.5°C at 1 bar, higher temperatures are not feasible.

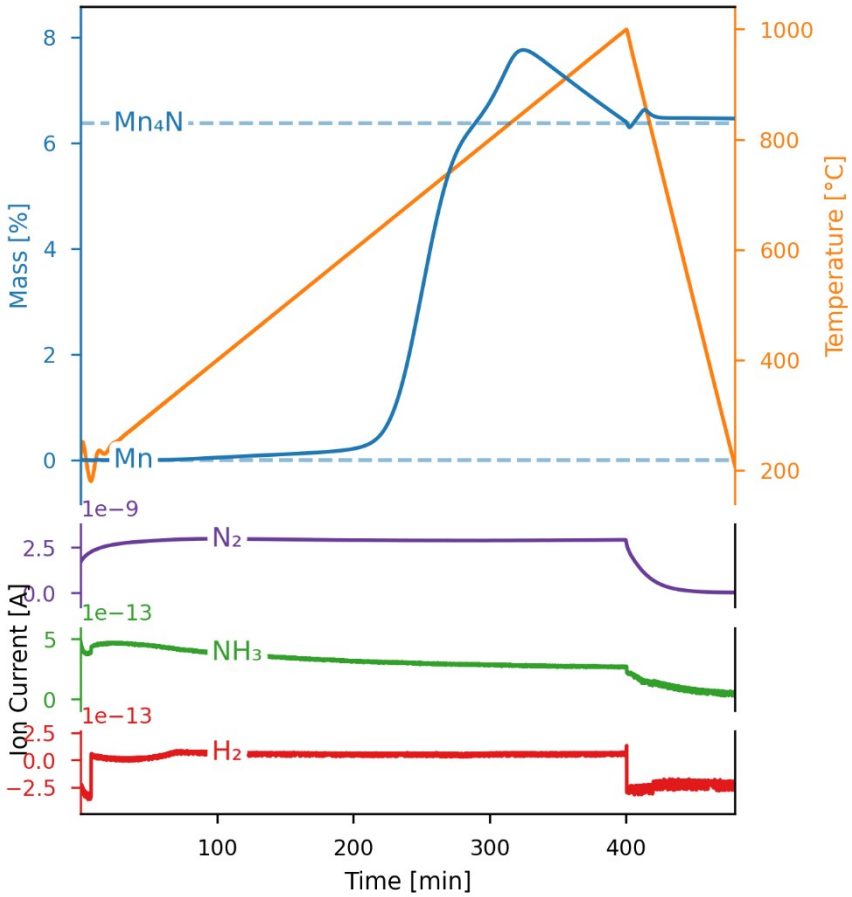

Figure S145: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Mn-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%) and full conversion to Mn_4N (6.37%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 200-1000°C at a rate of 2°C/min in 100% N_2 and cooled down back to 200°C in 100% Ar. Mn reacted to Mn_4N, in agreement with the Ellingham diagram (Figure S70).

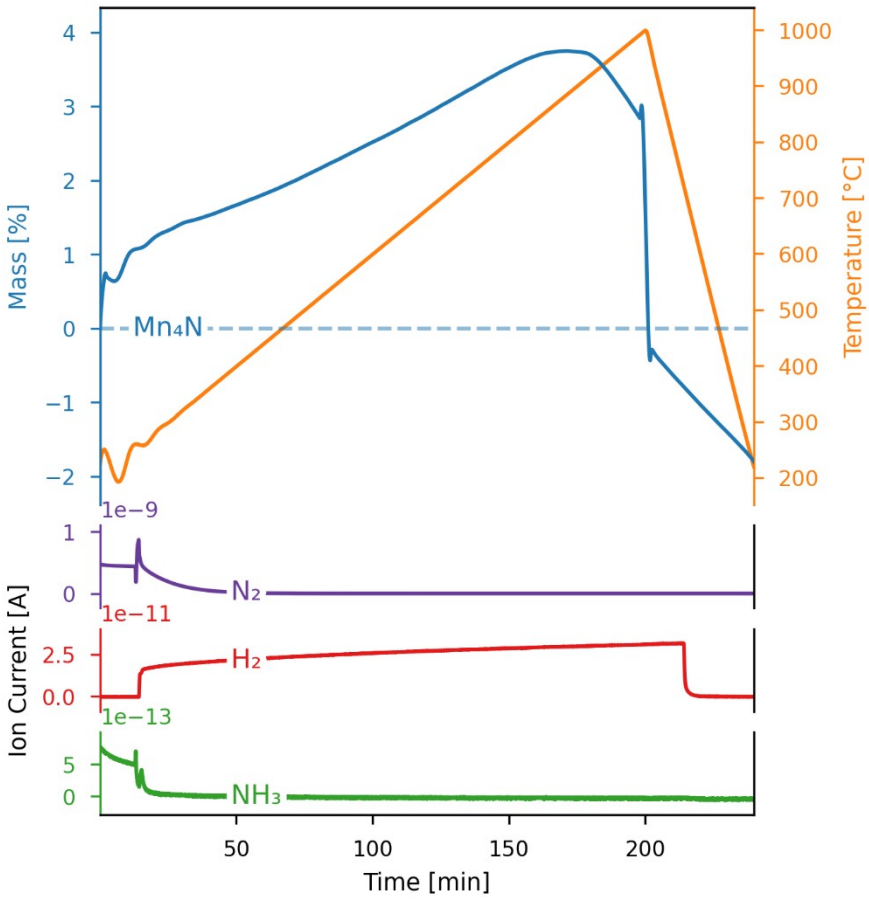

Figure S146: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Mn_4N-hydrogenation under 5% H. in Ar. Blue dashed lines: theoretical mass changes for no conversion (0%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 200-1000°C at a rate of 4°C/min in 5% H_2 in Ar and cooled down back to 200°C in 100% Ar. A mass increase was measurable up until 900°C, above that the mass decreases. The Ellingham diagram (Figure S77) and none of the reactions (Table S21) can help explain this behaviour.

The Mo-based system

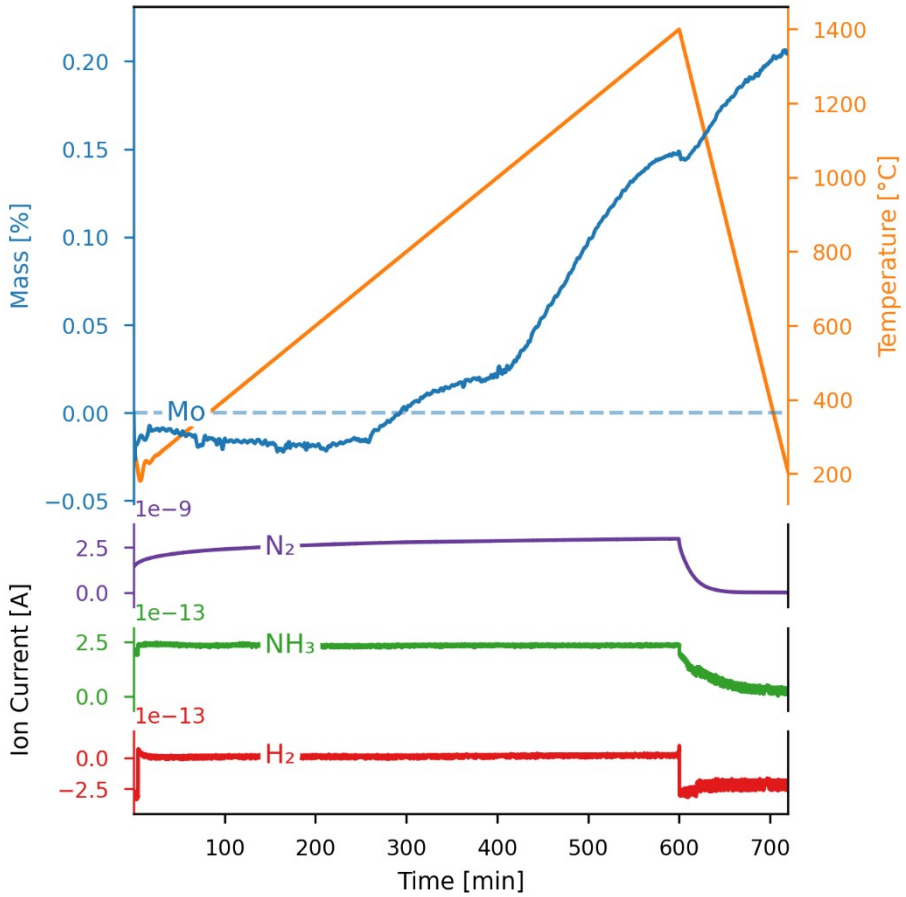

Figure S147: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Mo-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 200-1400°C at a rate of 2°C/min in 100% N_2 and cooled down back to 200°C in 100% Ar. No significant reaction was measurable. According to the Ellingham diagram (Figure S80), the formation of Mo_2N should be favourable below 680°C.

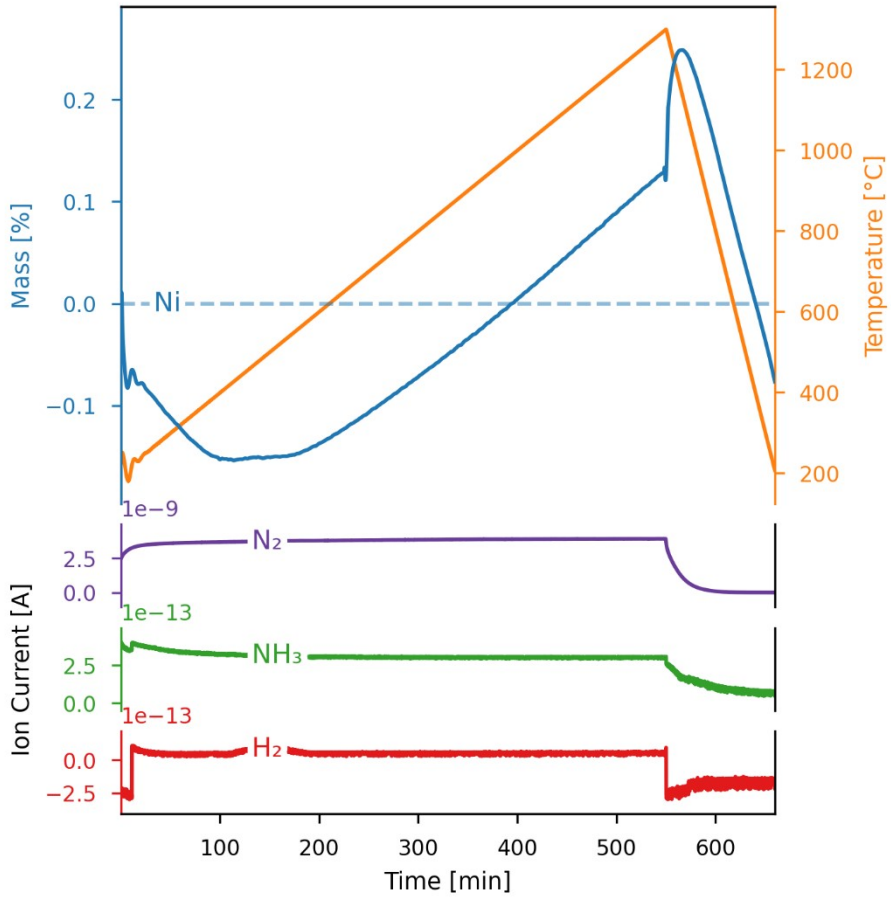

Figure S148: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Ni-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 200-1300°C at a rate of 2°C/min in 100% N_2 and cooled down back to 200°C in 100% Ar. No significant reaction was measurable, in agreement with the Ellingham diagram (Figure S92).

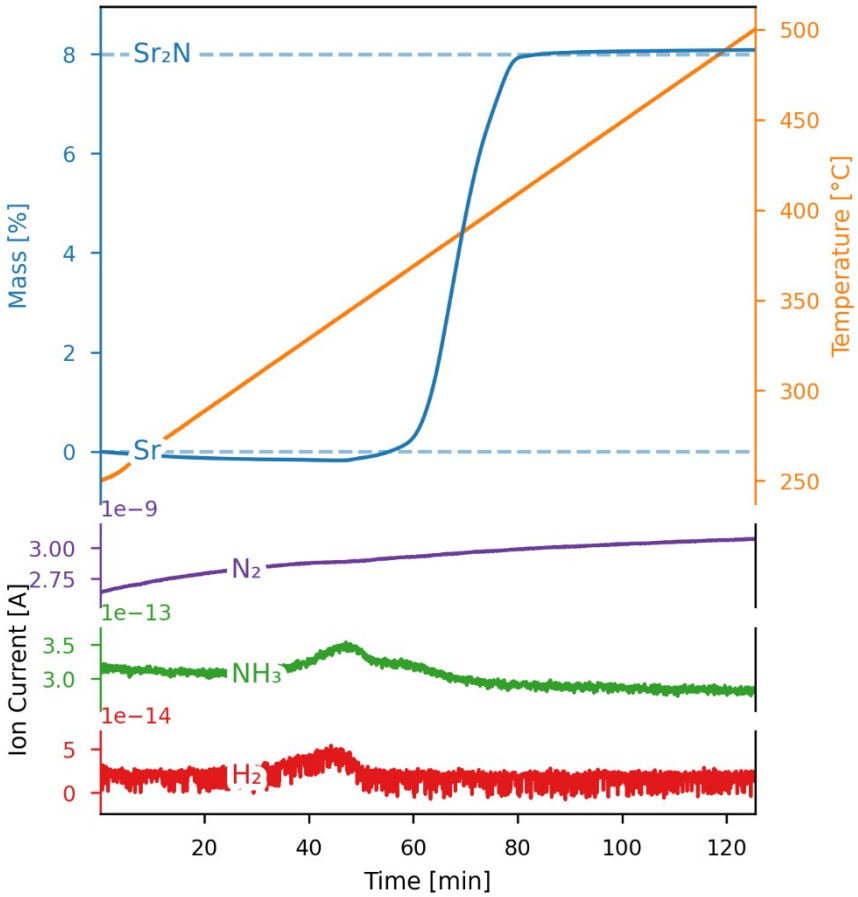

Figure S149: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Sr (granules)-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%) and full conversion to Sr_2N (7.99%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 200-500°C at a rate of 2°C/min in 100% N_2. Sr reacted to Sr_2N, in agreement with the Ellingham diagram (Figure S106).

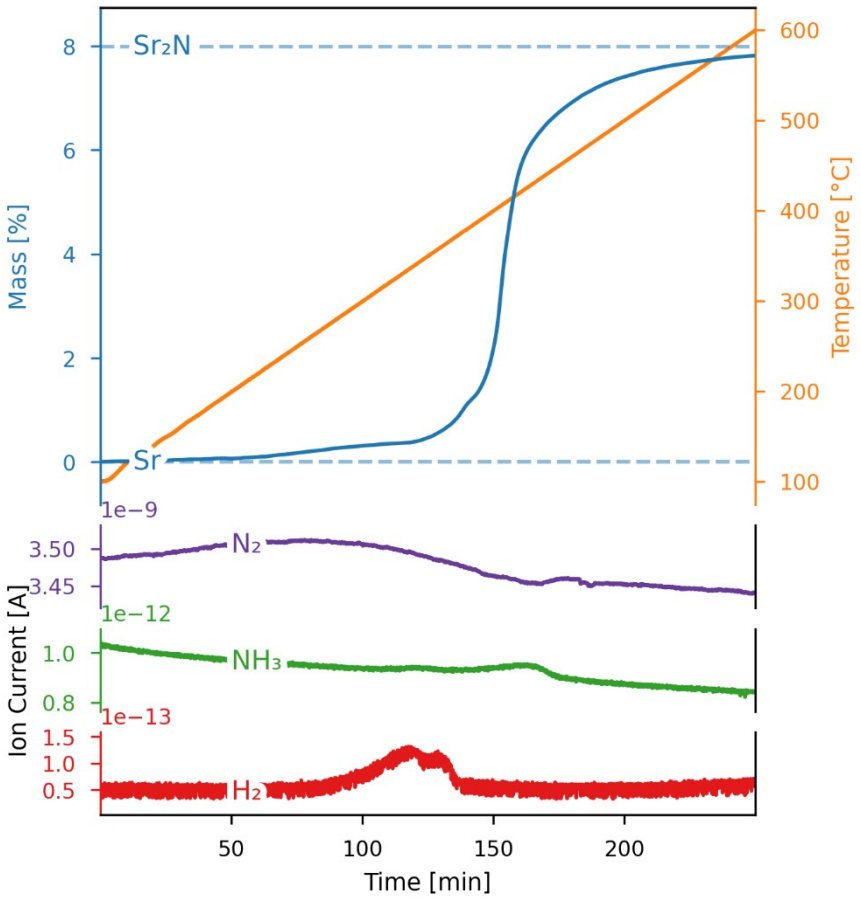

Figure S150: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Sr (random pieces)-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%) and full conversion to Sr_2N (7.99%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 100-600°C at a rate of 2°C/min in 100% N_2. Sr reacted to Sr_2N, in agreement with the Ellingham diagram (Figure S106). This TGA run is also shown in Figure 6.

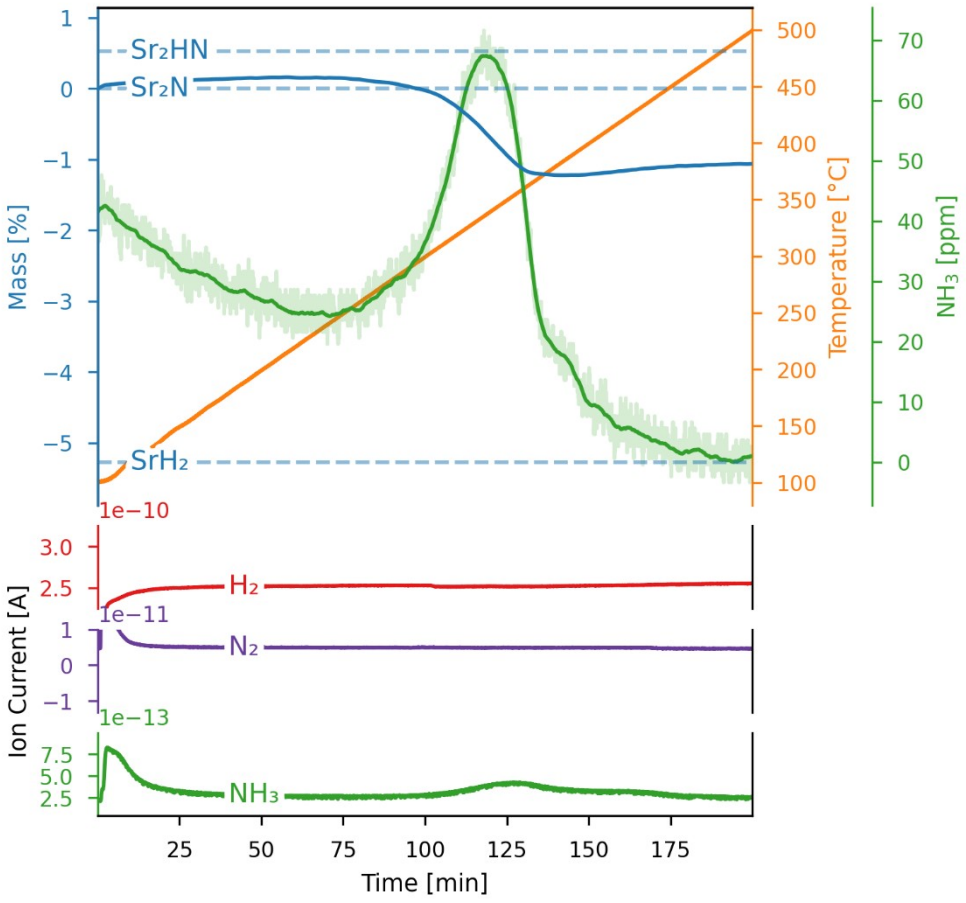

Figure S151: Variations of mass and temperature (recorded by the TGA), ion current (recorded by the mass spectrometer), and NH_3 concentration (recorded by the NH_3 analyzer) as a function of time for the Sr-nitridation under 5% H_2 in Ar Blue dashed lines: theoretical mass changes for no

conversion (0%), full conversion to SrH_2 (-5.27%), and full conversion to Sr_2HN (0.53%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 100-500°C at a rate of 2°C/min in 5% H_2 in Ar. Sr reacted to a mixture of Sr_2HN and SrH_2 in agreement with the Ellingham diagrams (Figure S114 and Figure S115). The NH_3 peak reached its maximum at 339°C. This TGA run is also shown in Figure 7.

The W-based system

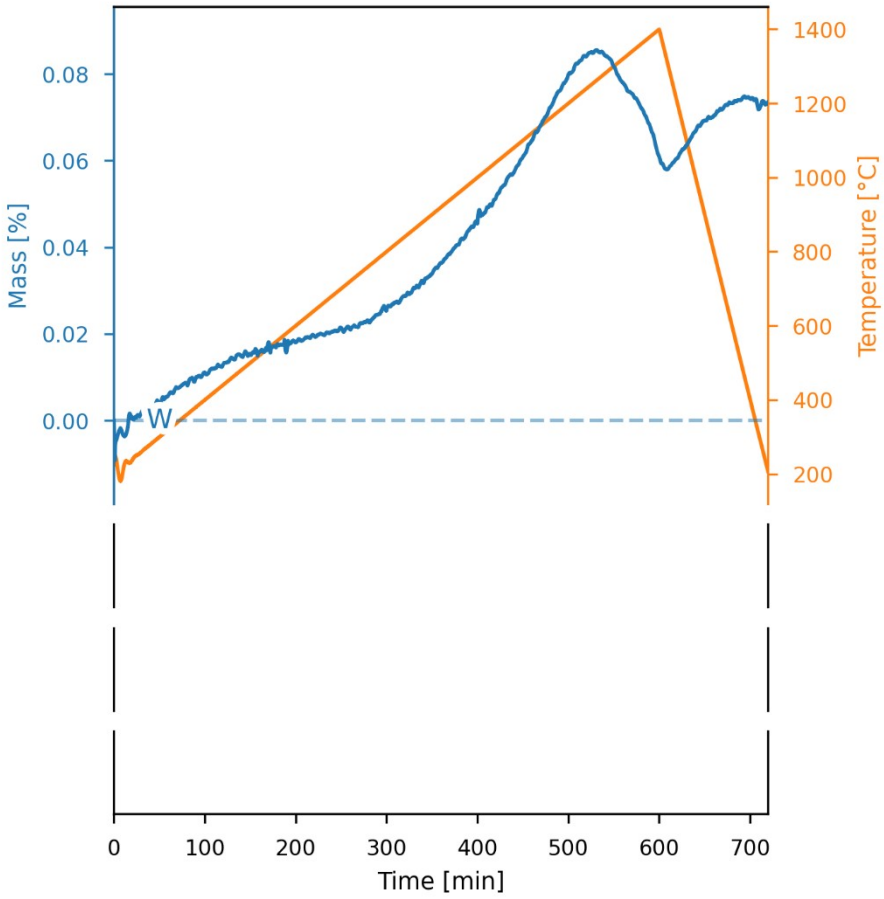

Figure S152: Variations of mass and temperature (recorded by the TGA) as a function of time for the W-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%). Sample was heated from 200-1400°C at a rate of 2°C/min in 100% N_2 and cooled down back to 200°C in 100% Ar. No significant reaction was measurable. According to the Ellingham diagram (Figure S120), the formation of W_2N should be favourable in this temperature range.

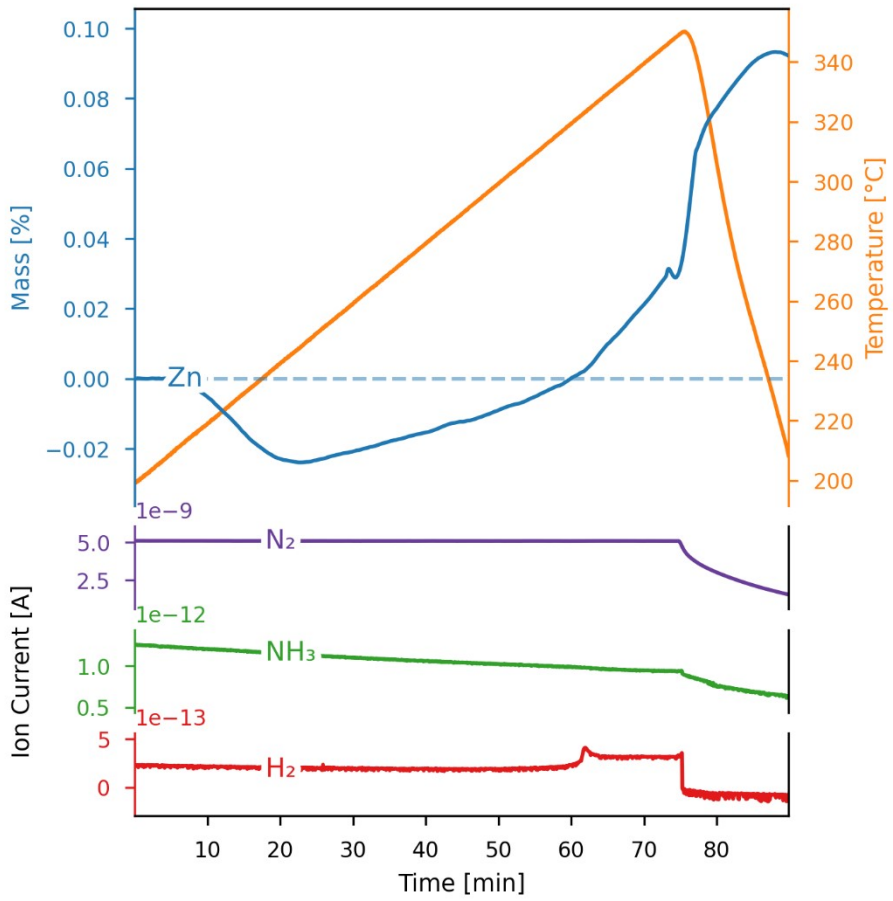

Figure S153: Variations of mass and temperature (recorded by the TGA) and ion current (recorded by the mass spectrometer) as a function of time for the Zn-nitridation under 100% N_2. Blue dashed lines: theoretical mass changes for no conversion (0%). The ion current signals correspond to N_2 (purple), NH_3 (green), and H_2 (red). Sample was heated from 200-350°C at a rate of 2°C/min in 100% N_2 and cooled down back to 200°C in 100% Ar. No significant reaction was measurable, in agreement with the Ellingham diagram (Figure S128).

2.1 Converting ppm to mg/s for mass balance

The NH_3 concentration $c_{NH_3,ppm}$ in ppm was recorded by the ABB Advance Optima AO2020 analyzer. The gas flow properties, temperature T in K, pressure P in Pa, and volumetric flow $\dot{V}$ in ml/min, were recorded by the Mesa Labs DryCal Defender 530+ Low Flow flow meter.

By definition, the concentration $c_{NH_3,ppm}$ is defined as the moles of NH_3 n_{NH_3} over 1'000'000 moles in the total gas flow n_{gas}, i.e. $1\ ppm\ of\ NH_3 = \frac{1\ mol\ of\ NH_3}{1'000'000\ moles\ of\ gas}$. The mass of NH_3 m_{NH_3} in g is calculated as

$$m_{NH_3} = n_{NH_3} \cdot M_{NH_3}$$

where M_{NH_3} is the molar mass of NH_3 in g/mol. The volume V in m^3 that 1'000'000 moles of gas occupy is calculated according to the ideal gas law:

$$V = \frac{1'000'000\ mol \cdot R \cdot T}{P}$$

where R is the universal gas constant in J/mol/K.

The mass flow of NH_3 $\dot{m}_{NH_3}$ in mg/s is then given as:

$$\dot{m}_{NH_3} = \frac{m_{NH_3} \cdot 1000\ \frac{mg}{g}}{V \cdot 1'000'000\ \frac{ml}{m^3}} \cdot \frac{\dot{V}}{60\ \frac{s}{min}}$$

2.2 Solid Characterization by XRD

Figure S154 shows the XRD pattern of Kapton tape. Patterns were obtained by a Bruker AXS D2 Phaser diffractometer operated at 30 kV and 10 mA (Cu Kα) at 2θ = 5–105°. The scanning step size and duration were 0.012° and 0.5 s, respectively. The background and Kα2 were stripped using Bruker's DIFFRAC.EVA V3.1.

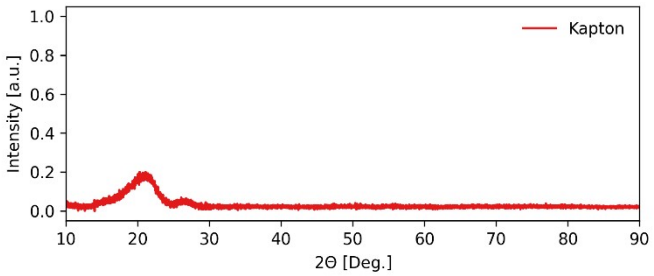

Figure S154: XRD patterns of Kapton tape. Peak intensities have been scaled to match with intensities observed in runs with a sample.

Figure S155 shows the XRD patterns of the Sr random pieces (Sigma-Aldrich, 99%, flakes in mm-range size). The sample was enclosed between two layers of Kapton tape. Patterns were obtained by a Bruker AXS D8 Advance diffractometer operated at 40 kV and 30 mA (Cu Kα) at 2θ = 10–100°. The scanning step size and duration were 0.01° and 0.5 s, respectively. The background and Kα2 were stripped using Bruker's DIFFRAC.EVA V7.0.

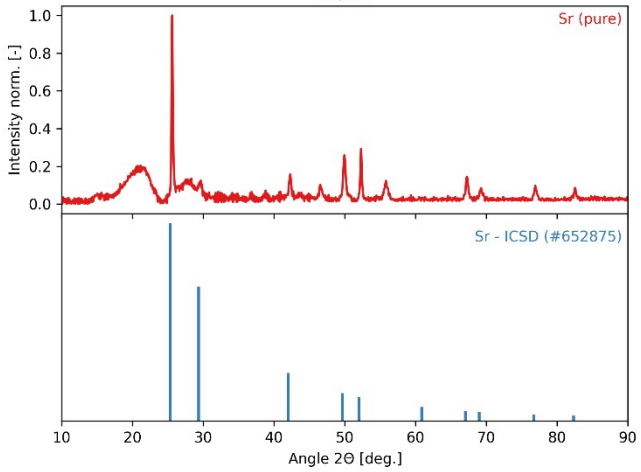

Figure S155: XRD patterns of the pure Sr. Peak intensities have been normalized.

3. References

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