Supporting Information

Conversion of Dinitrogen to Ammonia on Ru Atom Supported on Boron Sheets: A DFT Study

Chuangwei Liu,[ab] Qinye Li,[c] Jie Zhang,[b] Yonggang Jin,[d] Douglas MacFarlane[b] Chenghua Sun*[ae]

[a] Science & Technology Innovation Institute, Dongguan University of Technology, Dongguan, China

[b] School of Chemistry, Faculty of Science, Monash University, Clayton, Victoria 3800, Australia

[c] School of Chemical Engineering, Monash University, Clayton, Victoria 3800, Australia

[d] CSIRO Energy, 1 Technology Court, Pullenvale, Queensland 4069, Australia

[e] Department of Chemistry and Biotechnology, Faculty of Science, Engineering & Technology, Swinburne University of Technology, Hawthorn, Victoria 3122, Australia

Email: chenghuasun@swin.edu.au

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Thermochemistry

The fundamental thermodynamic relation states that

$$G^0 = H^0 - TS \quad (1)$$

At constant pressure and ambient temperature, the enthalpy can be described as term of H^0 and the heat capacity, C_P:

$$H = H^0 + \int C_P \, dT \quad (2)$$

Moreover, the entropy term can be presented to the sum of the translational, rotational, vibrational, and electronic contributions as to:

$$S = S_t + S_r + S_v + S_e \quad (3)$$

In the above equation, the approximations entropy can be expressed:

(a) At the fundamental electronic level: $S_e = 0$.
(b) For gases, translational, rotational, and vibrational entropy terms have contributions that might not be neglected: $S = S_t + S_r + S_v$.
(c) For solids and adsorbates, both $S_t = 0$ and $S_r = 0$, and thus: $S = S_v$.
(d) Because $\int C_P \, dT$ is almost negligible and $\Delta \int C_P \, dT = 0$, no thermal corrections for the enthalpy have been taken into the following calculate for Gibbs free energies (ΔG).

And also, intrinsic zero point energy (ZPE) and extrinsic dispersion (D) corrections can be obtained by the above analytical:

$$G = H^0 + \int C_P \, dT - T(S_t + S_r + S_v + S_e) + ZPE + D \quad (4)$$

The neighboring intermediates can be named as 1 and 2, thus we can gain the Gibbs free energy of neighboring intermediates reaction:

$$\Delta G_{21} = G_2 - G_1 \quad (5)$$

Such as: in the reaction (N_2*→N_2H*), the Gibbs free energy $\Delta G = G(N_2H^*) - G(N_2^*) - G(H^+/e^-)$

In such equation, the chemical potential of the H+/e- pair has the half value of the chemical potential of the dihydrogen molecule, under the standard hydrogen electrode conditions, the $G(H^+/e^-)$ equal to ½ $G(H_2)$.

Table S1. The system energy (eV), binding energy (eV) and cohesive energy (eV) of the TM-embedded α sheet and distance of transition single metal (TM) to monolayer (Å).

Metal Atoms	System Energy (eV)	Binding Energy (eV)	Cohesive Energy (eV)	Distance of TM to Substrates (Å)
Ti	-205.77	-4.01	5.54	1.60
Mn	-206.10	-2.43	3.39	1.38
Fe	-205.38	-4.04	4.79	1.08
Co	-203.76	-4.79	5.11	0.80
Ni	-202.38	-4.32	4.74	0.88
Cu	-201.42	-2.42	3.55	1.30
Nb	-209.04	-4.53	7.07	1.66
Mo	-210.37	-3.28	6.57	1.49
Ru	-206.93	-6.49	6.84	1.26
W	-213.21	-4.61	8.4	1.53

Table S2. The system energy (eV) and binding energy (eV) of the TM-embedded of β_{12} sheet and distance of TM to monolayer (Å).

Metal Atoms	System Energy (eV)	Binding Energy (eV)	Distance of TM to Substrates (Å)
Ti	-191.08	-5.28	1.40
Mn	-192.19	-2.91	0.91
Fe	-191.69	-4.30	0.90
Co	-190.47	-4.66	0.44
Ni	-188.87	-4.41	0.66
Cu	-187.81	-2.61	1.24
Nb	-195.87	-4.30	1.33
Mo	-197.13	-3.09	1.15
Ru	-193.43	-6.53	1.09
W	-199.85	-4.55	1.15

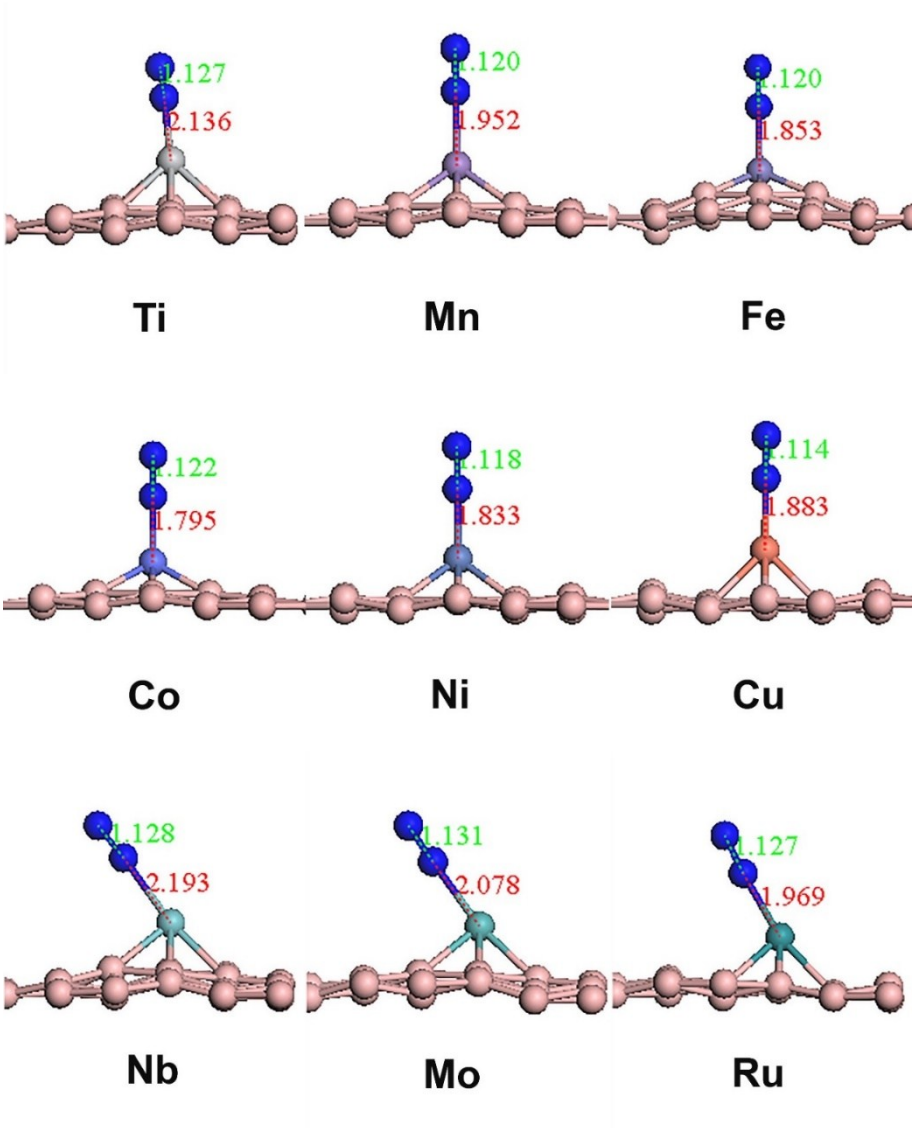

Figure S1. Optimized structures of N_2 adsorption on single TM-embedded α sheet.

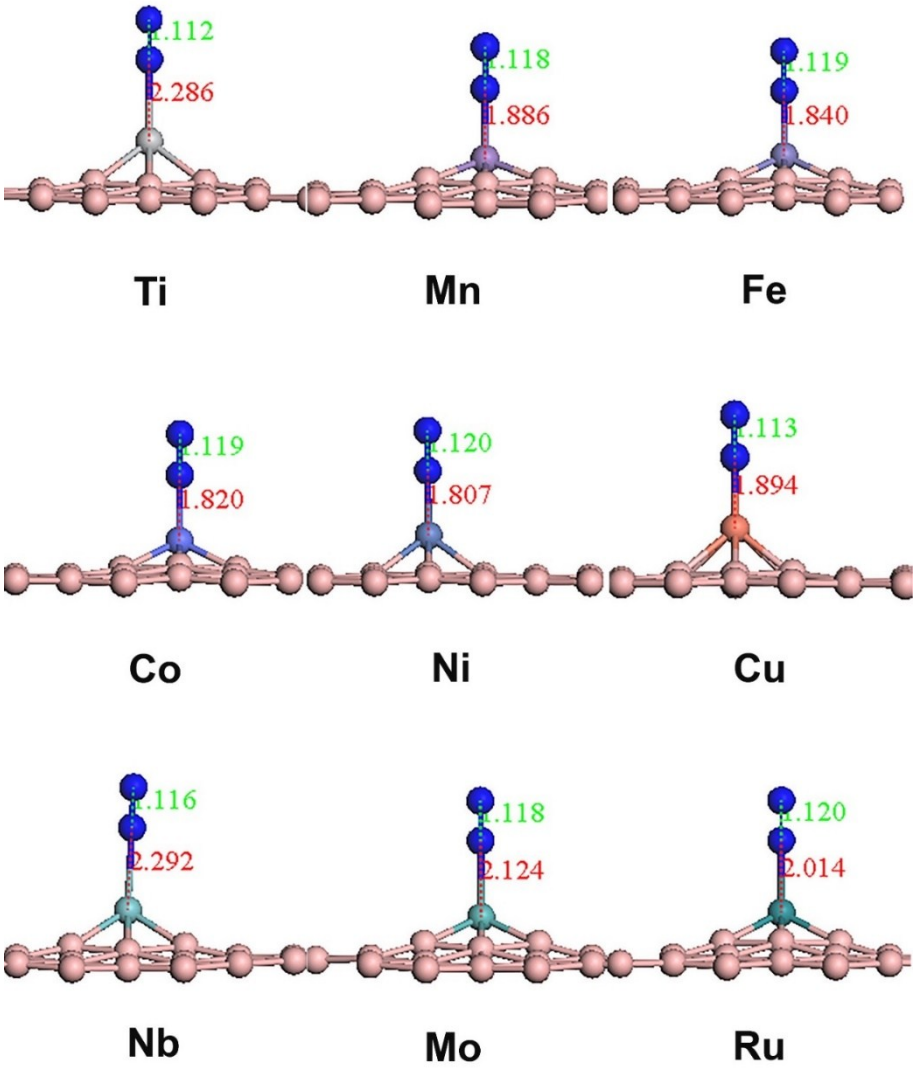

Figure S2. Optimized structures of N_2 adsorption on single TM-embedded β_{12} sheet.

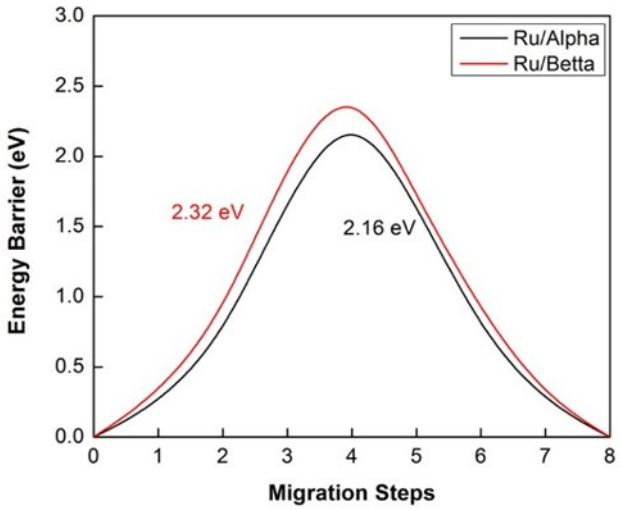

Figure S3. The energy barrier of a single Ru atom migration between two holes of two boron sheets.

Table S3. The N-N, B-N bond length (Å), and the Gibes free energies (ΔG, eV) of the adsorbed N_xH_y species on the Ru-embedded α sheet by two reaction pathways (distal and alternating pathways). 1 represents the adsorbed N_2*.

Reaction Step		1	2	3	4	5	6	7
Distal	ΔG	0.11	0.42	0.18	-0.94	-0.01	-0.42	0.26
	N-N	1.13	1.23	1.33	3.52			
	B-N	1.97	1.81	1.80	1.65	1.77	1.94	
Alternating	ΔG	0.11	0.42	0.66	-0.18	0.07	-1.75	0.26
	N-N	1.13	1.23	1.29	1.42	1.78	3.60	
	B-N	1.97	1.81	1.99	1.93	1.76	1.94	

Table S4. The N-N, B-N bond length (Å), and the Gibes free energies (ΔG, eV) of the adsorbed N_xH_y species on the Ru-embedded β_{12} sheet by two reaction pathways (distal and alternating pathways). 1 represents the adsorbed N_2*.

Reaction Step		1	2	3	4	5	6	7
Distal	ΔG	0.04	0.44	0.23	-1.24	0.13	-0.27	0.25
	N-N	1.12	1.23	1.33	3.49			
	B-N	2.01	1.79	1.76	1.64	1.74	1.91	
Alternating	ΔG	0.04	0.44	0.81	-0.37	1.19	-2.78	0.25
	N-N	1.12	1.23	1.29	1.42	1.48	3.61	
	B-N	2.01	1.79	1.99	1.91	1.75	1.91	

Cartesian Coordinates

Clear Ru-embedded α boron sheet

B1	0.331952	0.163903	0.488469
B2	0.163905	0.331975	0.488513
B3	0.331893	0.331897	0.495623
B4	0.165066	0.999702	0.498890
B5	0.999698	0.165106	0.498926
B6	0.164885	0.164879	0.506187
B7	0.334628	0.999706	0.498877
B8	0.999690	0.334644	0.498916
B9	0.833345	0.166700	0.508396
B10	0.668079	0.331960	0.488468
B11	0.834948	0.334639	0.498889
B12	0.665390	0.000332	0.498959
B13	0.500017	0.164885	0.506147
B14	0.665402	0.165090	0.498875
B15	0.834944	0.000341	0.498963
B16	0.500009	0.331902	0.495575
B17	0.331961	0.668071	0.488558
B18	0.166680	0.833369	0.508397
B19	0.334639	0.834968	0.498961
B20	0.164877	0.500020	0.506273
B21	0.000326	0.665407	0.498933
B22	0.165078	0.665400	0.498963
B23	0.331879	0.500014	0.495749
B24	0.000322	0.834962	0.498920
B25	0.836113	0.668083	0.488516
B26	0.668053	0.836123	0.488560
B27	0.835148	0.835154	0.506278
B28	0.668129	0.500002	0.495626
B29	0.500014	0.668163	0.495781
B30	0.668146	0.668138	0.495754
B31	0.835147	0.500020	0.506192
B32	0.500006	0.835150	0.506336
Ru1	0.500012	0.499918	0.562974

N_2*

B1	0.326007	0.160578	0.489140
B2	0.155952	0.327814	0.487399
B3	0.325269	0.328627	0.493283
B4	0.158108	0.995541	0.490790
B5	0.993349	0.162164	0.503310
B6	0.158068	0.161440	0.502878
B7	0.327362	0.995551	0.489497
B8	0.993338	0.330790	0.503356
B9	0.825062	0.162357	0.512750
B10	0.661894	0.329127	0.490010
B11	0.827681	0.332055	0.507387
B12	0.658533	0.996293	0.507011
B13	0.492573	0.160255	0.504922
B14	0.658555	0.161883	0.507065
B15	0.827652	0.995230	0.507255
B16	0.492892	0.326997	0.499593
B17	0.325990	0.665082	0.489153
B18	0.159058	0.829334	0.503456
B19	0.327372	0.831462	0.489441
B20	0.158047	0.496254	0.502750

B21	0.993290	0.662021	0.493184
B22	0.158096	0.662231	0.490713
B23	0.325190	0.496275	0.493137
B24	0.993261	0.830896	0.493206
B25	0.827208	0.663425	0.494423
B26	0.661845	0.832411	0.489903
B27	0.828484	0.832012	0.509854
B28	0.660271	0.495458	0.504500
B29	0.492846	0.665457	0.499450
B30	0.660222	0.664369	0.504322
B31	0.828534	0.496115	0.509872
B32	0.492576	0.831942	0.504838
Ru1	0.488675	0.494352	0.569687
N1	0.599643	0.552263	0.655050
N2	0.655617	0.581438	0.705706

N_2H*

B1	0.333421	0.165398	0.492185
B2	0.166235	0.333139	0.491337
B3	0.328633	0.327741	0.512173
B4	0.166016	0.999928	0.492156
B5	0.000037	0.165388	0.492657
B6	0.163664	0.163707	0.504362
B7	0.334643	0.999584	0.492278
B8	0.000037	0.334688	0.492648
B9	0.834226	0.167132	0.500908
B10	0.667823	0.332576	0.492423
B11	0.835288	0.334614	0.491970
B12	0.666741	0.001139	0.492368
B13	0.500686	0.163099	0.503813
B14	0.666743	0.165640	0.492348
B15	0.835287	0.000711	0.491999
B16	0.500687	0.327290	0.512116
B17	0.333422	0.668061	0.492213
B18	0.167207	0.833624	0.501019
B19	0.334645	0.835096	0.492293
B20	0.163658	0.499994	0.504374
B21	0.001267	0.666049	0.492958
B22	0.166018	0.666129	0.492177
B23	0.328623	0.500929	0.512203
B24	0.001263	0.835256	0.492951
B25	0.835079	0.667559	0.491691
B26	0.667816	0.835277	0.492447
B27	0.837644	0.836940	0.504626
B28	0.672831	0.499791	0.513166
B29	0.500682	0.673443	0.512180
B30	0.672836	0.673077	0.513200
B31	0.837645	0.500742	0.504603
B32	0.500688	0.837628	0.503847
Ru1	0.499265	0.499618	0.575614
N1	0.489360	0.494542	0.665536
N2	0.465096	0.482327	0.726250
H1	0.562470	0.531135	0.754504

N_2H_2*

B1	0.316320	0.152708	0.493494
B2	0.148042	0.320964	0.490597
B3	0.313910	0.318684	0.506756

B4	0.148835	0.988049	0.491352
B5	0.983501	0.154123	0.499577
B6	0.148225	0.153048	0.505589
B7	0.317642	0.987646	0.490010
B8	0.983397	0.322830	0.498944
B9	0.816934	0.155230	0.510026
B10	0.652203	0.321774	0.492168
B11	0.818522	0.323769	0.502814
B12	0.649238	0.988606	0.504217
B13	0.483019	0.151550	0.507787
B14	0.649335	0.154194	0.503886
B15	0.818621	0.988222	0.503965
B16	0.483233	0.316707	0.509983
B17	0.316343	0.657163	0.493079
B18	0.150060	0.821855	0.503993
B19	0.317738	0.823569	0.490365
B20	0.147925	0.488601	0.505397
B21	0.983771	0.654274	0.495003
B22	0.148981	0.654502	0.491499
B23	0.313551	0.488808	0.506973
B24	0.983763	0.823205	0.495346
B25	0.818049	0.655793	0.495384
B26	0.651994	0.823798	0.492838
B27	0.820581	0.825479	0.513246
B28	0.654613	0.487971	0.513807
B29	0.482920	0.660042	0.510998
B30	0.654717	0.660010	0.514363
B31	0.820450	0.488473	0.512096
B32	0.483023	0.825123	0.508508
Ru1	0.485868	0.490050	0.576399
N1	0.540696	0.523481	0.662983
N2	0.656866	0.589484	0.705273
H1	0.630408	0.601418	0.753445
H2	0.757625	0.675897	0.686415

N*

B1	0.332208	0.164247	0.489554
B2	0.164334	0.332157	0.489619
B3	0.330210	0.330137	0.506023
B4	0.165267	0.999711	0.494053
B5	0.999783	0.165209	0.494083
B6	0.163960	0.163891	0.504599
B7	0.334608	0.999703	0.494020
B8	0.999787	0.334554	0.494088
B9	0.833439	0.166705	0.503872
B10	0.668015	0.332133	0.489490
B11	0.834951	0.334535	0.493978
B12	0.665604	0.000374	0.494059
B13	0.500104	0.163883	0.504482
B14	0.665611	0.165198	0.494000
B15	0.834943	0.000382	0.494032
B16	0.500116	0.330152	0.505905
B17	0.332220	0.667928	0.489620
B18	0.166772	0.833372	0.503872
B19	0.334615	0.834874	0.494078
B20	0.163957	0.500036	0.504656
B21	0.000459	0.665550	0.493992
B22	0.165275	0.665531	0.494102
B23	0.330204	0.500040	0.506090

B24	0.000454	0.834885	0.494002
B25	0.835925	0.667952	0.489495
B26	0.668002	0.835837	0.489560
B27	0.836268	0.836199	0.504491
B28	0.669995	0.500039	0.505855
B29	0.500115	0.669944	0.506039
B30	0.670001	0.669927	0.505923
B31	0.836267	0.500036	0.504429
B32	0.500103	0.836191	0.504601
Ru1	0.500291	0.500031	0.573693
N1	0.500735	0.500027	0.656055

NH*

B1	0.335545	0.166762	0.489941
B2	0.168468	0.334306	0.490756
B3	0.332450	0.330622	0.509664
B4	0.168767	0.001753	0.494489
B5	0.003501	0.167185	0.496134
B6	0.167101	0.165047	0.508537
B7	0.338224	0.001861	0.495759
B8	0.003520	0.336532	0.496202
B9	0.836774	0.168493	0.505087
B10	0.671030	0.333725	0.488291
B11	0.838300	0.336132	0.494020
B12	0.669026	0.002285	0.492643
B13	0.504209	0.166261	0.506357
B14	0.668998	0.166958	0.492794
B15	0.838313	0.002422	0.493796
B16	0.504183	0.331851	0.506716
B17	0.335523	0.668979	0.489782
B18	0.170202	0.835192	0.504874
B19	0.338203	0.836571	0.495649
B20	0.167192	0.502321	0.508415
B21	0.004355	0.667728	0.491753
B22	0.168759	0.667220	0.494310
B23	0.332542	0.502066	0.509486
B24	0.004364	0.836823	0.491818
B25	0.839656	0.669915	0.487926
B26	0.671091	0.837568	0.488198
B27	0.839348	0.837445	0.503162
B28	0.673996	0.502288	0.503315
B29	0.504200	0.672499	0.506364
B30	0.673965	0.671934	0.503115
B31	0.839384	0.502153	0.503342
B32	0.504191	0.838094	0.506082
Ru1	0.502064	0.501107	0.572556
N1	0.461934	0.479656	0.659069
H1	0.378713	0.435017	0.694740

NH_2*

B1	0.321125	0.158181	0.489555
B2	0.152231	0.326248	0.493665
B3	0.318546	0.324780	0.504876
B4	0.153739	0.994197	0.505256
B5	0.987307	0.159305	0.492926
B6	0.152216	0.158391	0.508820
B7	0.323746	0.995115	0.504258
B8	0.987284	0.328280	0.492958
B9	0.820002	0.160147	0.503572

B10	0.656847	0.327635	0.489725
B11	0.823200	0.329230	0.491920
B12	0.653437	0.994846	0.491326
B13	0.488273	0.158857	0.507209
B14	0.653439	0.158916	0.491307
B15	0.823208	0.994247	0.491887
B16	0.488495	0.326520	0.502792
B17	0.321007	0.663196	0.489594
B18	0.154516	0.827484	0.511913
B19	0.323683	0.828960	0.504185
B20	0.152233	0.494149	0.508721
B21	0.988299	0.659495	0.502654
B22	0.153745	0.659894	0.505181
B23	0.318550	0.494109	0.504746
B24	0.988329	0.829142	0.502614
B25	0.825296	0.662739	0.489088
B26	0.656838	0.829469	0.489658
B27	0.823749	0.830021	0.505118
B28	0.656550	0.494853	0.497438
B29	0.488412	0.662318	0.502801
B30	0.656489	0.661899	0.497552
B31	0.823805	0.494067	0.505149
B32	0.488298	0.829776	0.507169
Ru1	0.497010	0.498551	0.570080
N1	0.612310	0.553831	0.652427
H1	0.560523	0.529292	0.698348
H2	0.727573	0.608902	0.656990

Clear Ru-embedded β_{12} sheet

B1	0.000000	0.418293	0.496789
B2	0.165355	0.330518	0.499728
B3	0.000000	0.080545	0.488857
B4	0.164672	0.161410	0.491428
B5	0.000000	0.248790	0.493815
B6	0.320430	0.400319	0.524018
B7	0.500000	0.315471	0.519369
B8	0.331985	0.079456	0.483644
B9	0.500000	0.157099	0.487158
B10	0.331126	0.236643	0.496771
B11	0.679570	0.400319	0.524018
B12	0.834644	0.330518	0.499728
B13	0.668015	0.079456	0.483644
B14	0.835328	0.161410	0.491428
B15	0.668874	0.236643	0.496771
B16	0.000000	0.919455	0.488857
B17	0.164672	0.838590	0.491428
B18	0.000000	0.581707	0.496789
B19	0.165355	0.669482	0.499728
B20	0.000000	0.751210	0.493815
B21	0.331985	0.920544	0.483644
B22	0.500000	0.842901	0.487158
B23	0.320430	0.599681	0.524018
B24	0.500000	0.684529	0.519369
B25	0.331126	0.763357	0.496771
B26	0.668015	0.920544	0.483644
B27	0.835328	0.838590	0.491428
B28	0.679570	0.599681	0.524018
B29	0.834644	0.669482	0.499728
B30	0.668874	0.763357	0.496771
Ru1	0.500000	0.500000	0.554671

N_2*

B1	0.999983	0.418297	0.497743
B2	0.164872	0.332658	0.498169
B3	0.000002	0.081302	0.489402
B4	0.165036	0.162775	0.490474
B5	0.999997	0.249060	0.491875
B6	0.320614	0.407756	0.518402
B7	0.499961	0.317390	0.519260
B8	0.331442	0.079837	0.485499
B9	0.500028	0.157440	0.491473
B10	0.331107	0.239872	0.497915
B11	0.679426	0.407921	0.518330
B12	0.835092	0.332633	0.498143
B13	0.668555	0.079847	0.485503
B14	0.834970	0.162780	0.490456
B15	0.668902	0.239918	0.497939
B16	0.000002	0.918765	0.489394
B17	0.165035	0.837289	0.490456
B18	0.999983	0.581758	0.497734
B19	0.164867	0.667402	0.498147
B20	0.999997	0.750999	0.491866
B21	0.331439	0.920233	0.485483
B22	0.500028	0.842631	0.491440
B23	0.320583	0.592282	0.518372
B24	0.499960	0.682682	0.519196

B25	0.331109	0.760183	0.497876
B26	0.668557	0.920223	0.485487
B27	0.834971	0.837283	0.490438
B28	0.679457	0.592116	0.518301
B29	0.835096	0.667427	0.498122
B30	0.668900	0.760137	0.497900
Ru1	0.499963	0.500069	0.561071
N1	0.499830	0.500559	0.661756
N2	0.499758	0.500917	0.717750

N_2H*

B1	0.000733	0.413338	0.505003
B2	0.166220	0.330065	0.502712
B3	0.000333	0.076423	0.493087
B4	0.166501	0.158442	0.494356
B5	0.000622	0.245736	0.496693
B6	0.328079	0.410765	0.507507
B7	0.500774	0.323310	0.510463
B8	0.332142	0.075849	0.493062
B9	0.500319	0.155316	0.497409
B10	0.332370	0.239778	0.498479
B11	0.673613	0.410404	0.507378
B12	0.835298	0.330133	0.502414
B13	0.668604	0.075822	0.493278
B14	0.834454	0.158291	0.494630
B15	0.668737	0.239915	0.498595
B16	0.000190	0.913560	0.493574
B17	0.166632	0.831722	0.495727
B18	0.000562	0.577087	0.504547
B19	0.165933	0.659908	0.501427
B20	0.000291	0.744186	0.497937
B21	0.332328	0.914394	0.496078
B22	0.500382	0.834366	0.500191
B23	0.330324	0.579174	0.500077
B24	0.500236	0.663380	0.499003
B25	0.332389	0.749365	0.496191
B26	0.668052	0.914451	0.496200
B27	0.833947	0.831581	0.495388
B28	0.670734	0.579198	0.500862
B29	0.834784	0.659862	0.501156
B30	0.668053	0.749571	0.496109
Ru1	0.500746	0.498645	0.568902
N1	0.495121	0.543594	0.655228
N2	0.509179	0.564038	0.715638
H1	0.410558	0.553849	0.741407

N_2H_2*

B1	0.999959	0.418304	0.503608
B2	0.165638	0.335845	0.502460
B3	0.999934	0.081752	0.493865
B4	0.166279	0.164132	0.495863
B5	0.999947	0.251278	0.497089
B6	0.329813	0.415809	0.504112
B7	0.499920	0.328455	0.506649
B8	0.331520	0.080600	0.494280
B9	0.499931	0.159853	0.500378
B10	0.332160	0.244795	0.497739
B11	0.670063	0.415797	0.504348

B12	0.834249	0.335860	0.502543
B13	0.668335	0.080609	0.494283
B14	0.833575	0.164155	0.495813
B15	0.667705	0.244775	0.497762
B16	0.999945	0.918803	0.493805
B17	0.166323	0.836362	0.495711
B18	0.999990	0.582150	0.503481
B19	0.165740	0.664589	0.502229
B20	0.999968	0.749231	0.496996
B21	0.331593	0.919845	0.494215
B22	0.499945	0.840587	0.500053
B23	0.330095	0.584700	0.503699
B24	0.499965	0.671693	0.505845
B25	0.332205	0.755580	0.497460
B26	0.668293	0.919847	0.494220
B27	0.833585	0.836366	0.495650
B28	0.669903	0.584763	0.503911
B29	0.834227	0.664578	0.502249
B30	0.667712	0.755611	0.497467
Ru1	0.499936	0.499821	0.568651
N1	0.500285	0.496059	0.656575
N2	0.502288	0.481931	0.722716
H1	0.407816	0.512074	0.746780
H2	0.599147	0.510133	0.744494

N*

B1	0.999993	0.418190	0.504026
B2	0.165624	0.335158	0.501257
B3	0.999993	0.081065	0.492920
B4	0.166487	0.163634	0.494699
B5	0.999993	0.251008	0.496518
B6	0.329538	0.416603	0.500529
B7	0.499993	0.331653	0.502246
B8	0.332306	0.080951	0.494427
B9	0.499993	0.161029	0.499345
B10	0.332200	0.245373	0.496143
B11	0.670447	0.416603	0.500533
B12	0.834361	0.335158	0.501259
B13	0.667679	0.080951	0.494428
B14	0.833498	0.163634	0.494699
B15	0.667785	0.245373	0.496145
B16	0.999993	0.919009	0.492912
B17	0.166488	0.836439	0.494685
B18	0.999993	0.581885	0.504017
B19	0.165624	0.664914	0.501242
B20	0.999993	0.749066	0.496507
B21	0.332306	0.919123	0.494420
B22	0.499993	0.839044	0.499329
B23	0.329539	0.583469	0.500517
B24	0.499993	0.668419	0.502222
B25	0.332200	0.754699	0.496127
B26	0.667679	0.919123	0.494420
B27	0.833497	0.836439	0.494685
B28	0.670446	0.583469	0.500520
B29	0.834361	0.664914	0.501244
B30	0.667785	0.754699	0.496128
Ru1	0.499989	0.500050	0.568827
N1	0.499984	0.500074	0.650725

NH*

B1	0.997683	0.418030	0.504728
B2	0.164159	0.335224	0.502435
B3	0.999248	0.081000	0.492059
B4	0.165517	0.163902	0.494311
B5	0.998906	0.250984	0.497128
B6	0.328517	0.416702	0.499879
B7	0.498382	0.332114	0.499962
B8	0.331599	0.081081	0.495050
B9	0.498729	0.161219	0.500119
B10	0.331280	0.245143	0.495228
B11	0.667888	0.417320	0.496572
B12	0.832857	0.334905	0.501540
B13	0.666937	0.081211	0.496085
B14	0.832200	0.163892	0.496019
B15	0.666667	0.245542	0.495419
B16	0.999249	0.919133	0.492055
B17	0.165520	0.836229	0.494311
B18	0.997684	0.582100	0.504726
B19	0.164162	0.664907	0.502433
B20	0.998908	0.749147	0.497121
B21	0.331604	0.919051	0.495051
B22	0.498732	0.838917	0.500119
B23	0.328521	0.583428	0.499870
B24	0.498387	0.668014	0.499948
B25	0.331286	0.754986	0.495227
B26	0.666937	0.918919	0.496083
B27	0.832200	0.836240	0.496009
B28	0.667887	0.582816	0.496562
B29	0.832857	0.665224	0.501531
B30	0.666667	0.754587	0.495408
Ru1	0.499802	0.500070	0.565246
N1	0.505098	0.500108	0.652421
H1	0.444901	0.500298	0.695343

NH_2*

B1	0.000065	0.418245	0.505975
B2	0.165695	0.334259	0.502700
B3	0.000017	0.080942	0.493472
B4	0.166715	0.164278	0.497269
B5	0.000054	0.250257	0.499312
B6	0.330273	0.418191	0.493903
B7	0.500062	0.333832	0.496597
B8	0.333190	0.081417	0.497935
B9	0.500055	0.162762	0.501471
B10	0.332324	0.246340	0.494762
B11	0.669911	0.418157	0.493858
B12	0.834419	0.334273	0.502599
B13	0.666891	0.081396	0.497889
B14	0.833389	0.164266	0.497233
B15	0.667749	0.246292	0.494695
B16	0.000017	0.919231	0.493488
B17	0.166717	0.835893	0.497297
B18	0.000065	0.581927	0.505990
B19	0.165696	0.665915	0.502727
B20	0.000054	0.749916	0.499340
B21	0.333190	0.918757	0.497950
B22	0.500055	0.837415	0.501498
B23	0.330273	0.581986	0.493912

B24	0.500062	0.666342	0.496611
B25	0.332327	0.753835	0.494780
B26	0.666891	0.918778	0.497905
B27	0.833387	0.835906	0.497262
B28	0.669912	0.582020	0.493866
B29	0.834418	0.665901	0.502626
B30	0.667747	0.753882	0.494713
Ru1	0.500300	0.500087	0.563193
N1	0.498720	0.500224	0.658618
H1	0.404175	0.500357	0.687143
H2	0.592775	0.500381	0.686482