Supplementary Material for PCCP

New Insight into Selective Catalytic Reduction of Nitrogen Oxides by Ammonia over H-Form Zeolites: A Theoretical Study

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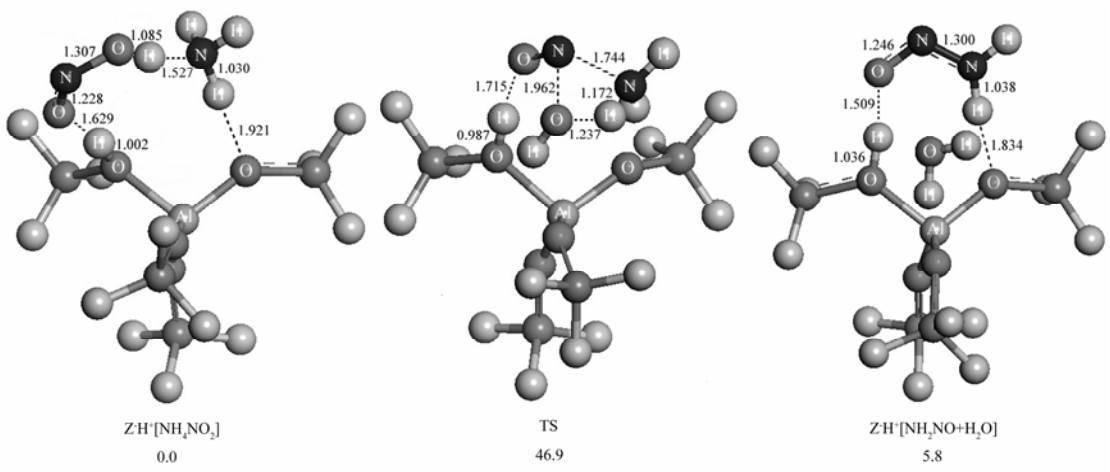

Fig. S1 Geometries and relative free energies of the reactant, transition state and product in the decomposition of NH_4NO_2 to NH_2NO and H_2O over the zeolitic cluster. Bond lengths are in Å. Free energies are in kcal/mol.

Table S1 Electronic Energies (kcal/mol) of *cis,trans*-HNNOH over the zeolitic cluster at different fixed N-O bond lengths. Bond lengths are in Å.

	N-O bond length	Electronic energy
Initial structure (Fig. 9)	1.419	-1895.345452
	1.450	-1895.346881
	1.500	-1895.348341
	1.550	-1895.349158
	1.600	-1895.351794
	1.650	-1895.363079
	1.700	-1895.373574
	1.900	-1895.406803
	2.100	-1895.426126
	2.300	-1895.449699
Decomposition product	3.150	-1895.459748

Table S2 Calculated Gibbs free energies at the temperature of 373 K for all species. The energy unit is kcal/mol.

Species	G_{373}	Species	G_{373}
N_2	-109.54255	ZH	-1709.42074
O_2	-150.34220	I	-1895.27769
NO	-129.90959	II	-1895.27138
NO_2	-205.09375	III	-1895.26346
NH_3	-56.54698	IV	-1895.26614
H_2O	-76.42153	V	-1895.26559
asym-N_2O_3	-334.99491	VI	-1895.26628
sym-N_2O_3	-334.99299	ZH[H_2O+N_2]	-1895.38645
trans,cis-N_2O_3	-334.99113	TSI/II	-1895.27000
sym-N_2O_4	-410.18324	TSIII/IV	-1895.25932
asym-N_2O_4	-410.17038	TSV/VI	-1895.25451
cis-HONO	-205.71249	trans,cis-HNNOH	-185.84518
trans-HONO	-205.71115	trans,trans-HNNOH	-185.84211
HNO_3	-280.89051	cis,trans-HNNOH	-185.84513
NH_2NO	-185.85082	Z[NH_4](2H)	-1765.98424
NH_2NO_2	-261.03203	Z[NH_4](3H)	-1765.97841
TS1	-410.13650	ZH[NH_4NO_2](a)	-1971.68107
TS2	-391.51502	TSa/c	-1971.60639
TS3	-391.51346	ZH[[NH_2NO+H_2O](c)	-1971.69026
TS4	-466.70222		
TS5	-486.57309		
TS6	-486.57528		

Coordinates and atomic charges for the optimized structures of all transition states in Fig. 2.

TS1

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	8	-0.135596	-0.595450	0.902623	0.515979
2	8	-0.135720	0.595397	0.902909	-0.515890
3	7	0.355240	1.521398	-0.059409	-0.317088
4	8	-0.219542	1.343067	-0.850811	0.542974
5	7	0.355297	-1.521374	-0.059279	0.316976
6	8	-0.219679	-1.343036	-0.850870	-0.542966

TS2

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	7	0.274901	-1.807279	-0.519195	-0.047781
2	8	-0.440879	-1.699492	0.761384	-0.123858
3	8	-0.353800	-0.748267	-1.145724	0.113829
4	7	0.250323	1.331876	-0.259772	0.470241
5	8	-0.111397	1.995669	-0.689131	-0.373360
6	7	-0.620563	0.738206	1.338374	0.029203
7	1	0.426552	-0.453206	1.112520	-0.046509
8	1	0.282678	1.206587	1.604836	-0.837459
9	1	0.292185	1.023716	1.954562	0.789425

TS3

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	8	-0.421165	-1.204583	1.082085	-0.244754
2	7	0.279790	-1.108471	-0.176174	0.057789
3	8	-0.321152	-2.111296	-0.846485	0.089257
4	7	0.215188	1.222474	-0.540709	0.474488
5	8	-0.138135	1.697252	-1.163407	-0.384618
6	7	-0.611003	1.235163	1.166541	0.076216
7	1	0.417682	0.053749	1.329929	-0.143071
8	1	0.294681	1.573861	1.644271	0.909435
9	1	0.284114	1.877235	1.300647	-0.704886

TS4

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	7	0.725824	-1.430427	-0.103401	-0.001654
2	8	-0.496093	-1.108158	1.132993	-0.210011
3	8	-0.447270	-0.503306	-0.932323	0.244587
4	7	0.270512	1.752925	-0.445909	0.441491
5	8	-0.082909	2.230804	-0.951254	-0.473751
6	7	-0.615927	1.390867	1.258602	0.097725
7	1	0.433406	0.247173	1.241006	-0.062358
8	1	0.292110	1.933175	1.550236	-0.715719
9	1	0.302396	1.672469	1.776690	0.928181
10	8	-0.382050	-2.600137	-0.441038	-0.049955

Coordinates and atomic charges for the optimized structures of all species in Fig. 8.

$Z^{-}H^{+}$

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	13	0.976327	-0.190888	-0.029318	-0.039306
2	8	-0.685209	-1.252064	-1.363967	-0.315032
3	8	-0.645075	0.736012	-0.246011	-1.737074
4	8	-0.692640	1.198340	-0.271284	0.960024
5	8	-0.638761	-0.883143	1.532997	-0.023789
6	14	0.666845	-2.532443	-2.317189	0.053988
7	1	-0.131873	-2.757712	-3.296091	-1.047051
8	1	-0.127032	-2.305078	-3.085499	1.310160
9	1	-0.124857	-3.784178	-1.527104	0.224533
10	14	0.710811	2.460940	-0.242010	-1.886593
11	1	-0.076877	3.042766	-1.424749	-1.224312
12	1	-0.096603	2.712008	-0.296383	-3.346385
13	1	-0.069201	2.899611	1.036433	-1.306916
14	14	0.673283	1.878565	-0.240024	2.452623
15	1	-0.129331	3.038370	-1.173577	2.496409
16	1	-0.126610	2.378897	1.121193	2.795666
17	1	-0.127434	0.913700	-0.652324	3.511022
18	14	0.659653	-1.582609	3.006692	-0.024272
19	1	-0.128099	-1.784271	3.508988	1.363559
20	1	-0.134081	-0.737786	3.997089	-0.751516
21	1	-0.129734	-2.913029	2.972907	-0.694947
22	1	0.376500	0.242741	-0.918192	-2.232709

I

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	13	2.133746	0.426138	-0.209738	-0.059746
2	8	-1.352646	-0.620425	-0.662729	1.291193
3	8	-1.300811	-0.548545	1.250218	-0.744281
4	8	-1.361543	0.493492	-1.405536	-1.283411
5	8	-1.336361	1.883884	0.592682	0.387582
6	14	1.484651	-0.348987	-1.086470	2.868679
7	1	-0.310791	-1.634688	-1.595020	3.427628
8	1	-0.295874	0.672817	-2.160309	2.985957
9	14	1.500788	0.108009	2.790007	-1.120000
10	1	-0.266758	-0.984453	3.523273	-1.798614
11	1	-0.264394	0.505977	3.487546	0.120091
12	1	-0.255287	1.254795	2.585888	-2.025354
13	14	1.586388	0.657683	-2.626954	-2.351257
14	1	-0.323817	-0.303442	-3.729088	-2.058361
15	1	-0.320530	0.394975	-2.157707	-3.741174
16	1	-0.318782	2.031164	-3.203276	-2.315589
17	14	1.548223	3.460430	0.711753	0.811798
18	1	-0.314813	4.354941	0.034352	-0.168559
19	1	-0.314305	3.858875	2.145339	0.879952
20	1	-0.318640	3.710860	0.104731	2.150085
21	7	-0.513915	-3.346463	-0.455543	0.693631
22	1	0.242726	-4.006703	-1.055365	1.169228
23	1	0.447688	-2.318856	-0.522965	0.873073
24	7	0.529797	-3.893271	0.397452	-0.121130
25	8	-0.691550	-3.107506	1.149603	-0.731738
26	1	0.685615	-1.568770	1.171326	-0.705039
27	1	-0.298805	0.083776	0.073905	3.692028

II

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	13	1.002206	0.399444	0.201432	-0.001473
2	8	-0.719216	-0.461510	-1.111461	-1.042365
3	8	-0.771450	-0.820335	0.361764	1.273590
4	8	-0.638943	0.569194	1.604792	-0.965120
5	8	-0.686930	1.815896	-0.657930	0.473054
6	14	0.706852	0.248973	-2.565573	-1.593404
7	1	-0.111112	-0.769446	-3.173488	-2.485558
8	1	-0.081603	1.469225	-2.220398	-2.346002
9	14	0.695533	-0.658901	0.440785	2.930297
10	1	-0.110034	-1.907335	1.013236	3.494823
11	1	-0.119776	-0.449983	-0.911132	3.513951
12	1	-0.118876	0.489547	1.304820	3.311581
13	14	0.665822	0.932346	2.982879	-1.760650
14	1	-0.132578	-0.012241	3.199007	-2.893195
15	1	-0.128350	0.845663	4.167630	-0.861575
16	1	-0.129431	2.311643	2.938007	-2.323346
17	14	0.663984	3.396896	-0.806346	0.876285
18	1	-0.126283	4.158912	0.450220	0.629917
19	1	-0.127012	3.546146	-1.157578	2.315810
20	1	-0.133725	4.029821	-1.891548	0.074608
21	7	-0.393646	-3.068255	-0.860824	-1.009134
22	1	0.289978	-3.612535	-1.334408	-1.734833
23	1	0.450450	-1.494073	-1.033940	-1.015487
24	7	0.124955	-3.887204	-0.184089	-0.340534
25	8	-0.386452	-3.371798	0.515452	0.653464
26	1	0.404240	-2.366001	0.391661	0.771835
27	1	-0.088605	0.534136	-3.471673	-0.462095

III

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	13	0.995921	-0.554896	-0.182639	-0.022389
2	8	-0.685708	0.334545	1.018123	-1.219918
3	8	-0.757856	0.863815	-0.940988	0.698889
4	8	-0.634717	-1.516489	-1.231803	-0.968297
5	8	-0.685197	-1.360285	1.003145	0.936414
6	14	0.714231	-0.033825	2.694092	-1.361153
7	14	0.696067	1.159260	-1.750076	2.118066
8	14	0.662394	-2.468036	-2.251014	-1.815206
9	14	0.666311	-2.407124	1.515387	2.087654
10	1	0.399430	1.265926	0.724696	-1.413797
11	1	-0.097251	0.776374	3.164917	-2.508755
12	1	-0.076801	-1.476164	2.790637	-1.642581
13	1	-0.086515	0.355255	3.413929	-0.131990
14	1	-0.117600	2.126467	-2.850084	1.869585
15	1	-0.121341	1.727663	-0.841206	3.148475
16	1	-0.125609	-0.101168	-2.332967	2.655905
17	1	-0.132475	-2.498438	-1.873574	-3.256954
18	1	-0.128673	-1.971746	-3.652978	-1.723202
19	1	-0.128187	-3.869245	-2.229587	-1.309485
20	1	-0.125104	-3.739867	0.861801	1.962746
21	1	-0.128394	-1.889015	1.235975	3.456724
22	1	-0.132540	-2.603678	2.987125	1.965737
23	7	-0.265054	4.221054	-0.069515	0.303146
24	7	0.078615	3.865275	0.292739	-0.822568
25	8	-0.460615	2.632895	-0.245829	-1.154726
26	1	0.282476	5.140247	0.368183	0.452478
27	1	0.394189	2.227022	-0.693744	-0.347824

IV

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	13	0.992963	-0.571347	0.054409	-0.001917
2	8	-0.764860	0.313674	1.533866	0.404732
3	8	-0.693213	0.795601	-0.858087	-0.978055
4	8	-0.639735	-1.886634	0.316985	-1.063217
5	8	-0.674527	-0.796246	-1.070740	1.282064
6	14	0.696307	-0.181926	2.965047	1.089380
7	14	0.707070	1.047858	-2.559876	-0.993048
8	14	0.657186	-3.165484	0.442490	-2.068171
9	14	0.665908	-1.443826	-1.650727	2.668686
10	1	0.399943	1.890343	1.470736	-0.233015
11	1	-0.113548	-0.445188	3.993133	0.047786
12	1	-0.120023	-1.422142	2.766387	1.887182
13	1	-0.116087	0.891235	3.470585	1.985649
14	1	-0.090258	1.894149	-2.837619	-2.174433
15	1	-0.089459	1.731801	-2.985414	0.245843
16	1	-0.078354	-0.290480	-3.161963	-1.125912
17	1	-0.127930	-3.375045	1.855926	-2.490089
18	1	-0.133789	-2.959957	-0.372777	-3.299698
19	1	-0.127747	-4.418999	-0.028819	-1.415399
20	1	-0.126305	-2.933208	-1.654063	2.630260
21	1	-0.131765	-0.988201	-3.051852	2.890490
22	1	-0.129740	-1.021381	-0.842832	3.847935
23	7	-0.242421	4.390482	-0.085495	-0.424934
24	7	0.045545	3.670222	0.785894	0.065005
25	8	-0.454180	2.583543	1.011222	-0.789565
26	1	0.283216	5.173611	-0.178282	0.236735
27	1	0.405802	1.603839	-0.276307	-1.092436

V

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	13	0.988557	0.595801	-0.153719	0.072706
2	8	-0.723176	-0.255890	-1.376419	-0.845835
3	8	-0.697763	-0.780493	1.148604	0.256584
4	8	-0.686363	1.732304	0.820464	-0.792979
5	8	-0.637098	1.038015	-0.646101	1.655087
6	14	0.682789	0.056937	-2.648132	-1.839369
7	1	-0.123936	0.582363	-2.211891	-3.163330
8	1	-0.124686	1.036153	-3.603805	-1.250415
9	14	0.708310	-0.583309	2.826394	-0.030126
10	1	-0.090639	-0.374337	3.093996	-1.468106
11	1	-0.102867	-1.850813	3.449525	0.420941
12	1	-0.082664	0.552121	3.283217	0.791247
13	14	0.664045	3.198313	1.096700	-1.464769
14	1	-0.129045	4.213558	1.479759	-0.442632
15	1	-0.131567	3.715084	-0.102296	-2.185894
16	1	-0.132418	3.105187	2.212228	-2.448315
17	14	0.660095	1.596998	-1.047094	3.130959
18	1	-0.130611	3.079889	-1.198726	3.136164
19	1	-0.136283	1.246514	-0.006759	4.141269
20	1	-0.133244	1.010011	-2.336106	3.597165
21	7	-0.314142	-2.892761	-0.367147	-0.183515
22	1	0.424354	-1.702812	0.741817	0.153708
23	1	0.332129	-2.442455	-1.219580	-0.540998
24	7	0.063666	-4.112438	-0.530467	-0.124216
25	8	-0.356646	-4.706231	0.617266	0.355488
26	1	-0.140709	-1.217608	-3.386318	-2.080170
27	1	0.349914	-5.648654	0.385913	0.367818

VI

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	13	0.988337	-0.580776	-0.182943	0.037905
2	8	-0.697457	0.387055	1.304706	0.729810
3	8	-0.720556	0.612083	-0.839684	-1.059193
4	8	-0.688557	-1.886865	0.707156	-0.664620
5	8	-0.637148	-0.956238	-1.198439	1.367925
6	14	0.711515	-0.225823	2.904204	0.805911
7	1	-0.089543	-0.415568	3.462365	-0.548315
8	1	-0.082041	-1.481411	2.863454	1.576247
9	14	0.681839	0.709849	-1.805073	-2.386016
10	1	-0.125417	0.161064	-1.142440	-3.602587
11	1	-0.137680	2.145191	-2.115005	-2.648184
12	1	-0.125871	-0.012892	-3.095299	-2.204402
13	14	0.665285	-3.327323	0.802320	-1.435625
14	1	-0.128791	-4.468878	0.759434	-0.478199
15	1	-0.131921	-3.419052	2.084412	-2.189496
16	1	-0.131298	-3.512442	-0.311789	-2.409828
17	14	0.660121	-1.442246	-2.204138	2.552887
18	1	-0.130734	-2.840884	-2.673037	2.338331
19	1	-0.133307	-0.569237	-3.410545	2.631026
20	1	-0.135326	-1.391115	-1.529605	3.882277
21	7	-0.315456	2.862868	0.517777	0.243941
22	1	0.312625	2.691753	-0.267440	-0.411543
23	1	0.428061	1.386236	1.169251	0.669391
24	7	0.096884	4.037899	0.718415	0.536672
25	8	-0.379071	4.891801	-0.173086	-0.102033
26	1	-0.105525	0.814917	3.675972	1.528100
27	1	0.351031	5.771944	0.087588	0.214810

$Z^{-}H^{+}[H_2O+N_2]$

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	13	0.979473	-0.578988	-0.119837	-0.003642
2	8	-0.754147	0.527988	-1.428216	0.427120
3	8	-0.708128	0.401919	0.625420	-1.444267
4	8	-0.679671	-0.624008	1.222014	1.075167
5	8	-0.639722	-2.059998	-0.690398	-0.653154
6	14	0.687117	0.894966	-2.266383	1.805751
7	14	0.720273	0.774354	2.279638	-1.675158
8	14	0.662309	-1.124360	2.094376	2.365965
9	14	0.665958	-3.583546	-1.071981	-1.090300
10	1	0.375936	1.441147	-1.732957	-1.073221
11	1	-0.121172	1.851425	-1.516483	2.664454
12	1	-0.121227	-0.323628	-2.557271	2.609362
13	1	-0.125504	1.531341	-3.556416	1.422760
14	1	-0.091439	1.645867	2.785432	-0.596669
15	1	-0.103159	1.472786	2.347261	-2.980514
16	1	-0.088284	-0.509144	3.006723	-1.722278
17	1	-0.129910	-0.694749	1.467700	3.648404
18	1	-0.131620	-0.540684	3.463716	2.309322
19	1	-0.127509	-2.607952	2.231420	2.403532
20	1	-0.128799	-4.466610	-1.260651	0.094916
21	1	-0.132835	-4.186595	-0.007294	-1.942409
22	1	-0.135037	-3.603400	-2.338834	-1.876948
23	7	0.008543	3.674428	0.311518	-0.256025
24	7	0.006315	4.466291	-0.200751	0.319985
25	8	-0.640927	1.724801	-1.461826	-1.981862
26	1	0.416756	1.003247	-0.101346	-1.842428
27	1	0.336410	1.303360	-2.083542	-2.590285

TSI/II

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	13	1.000779	0.368329	-0.066718	0.138077
2	8	-0.782443	-0.602258	1.487806	0.069635
3	8	-0.794834	-0.775785	-1.124443	-0.774324
4	8	-0.640794	0.504823	-0.576813	1.770259
5	8	-0.675649	1.803415	0.203415	-0.771815
6	14	0.700453	-0.028375	3.031817	-0.277214
7	1	-0.127448	-1.155973	3.959839	0.010966
8	1	-0.096575	1.122105	3.356476	0.595762
9	14	0.699917	-0.400253	-2.250646	-1.960744
10	1	-0.109005	-1.585226	-3.128592	-2.131089
11	1	-0.111988	-0.103249	-1.583639	-3.253435
12	1	-0.109797	0.768465	-3.066000	-1.547725
13	14	0.665427	0.942272	-1.094730	3.253734
14	1	-0.134583	0.070606	-0.487369	4.300183
15	1	-0.130242	0.819612	-2.575639	3.368363
16	1	-0.129572	2.351699	-0.729487	3.572563
17	14	0.658672	3.382938	0.207894	-1.193202
18	1	-0.128238	4.227943	-0.531499	-0.213018
19	1	-0.130629	3.572976	-0.427263	-2.527379
20	1	-0.133662	3.900312	1.603226	-1.278035
21	7	-0.392937	-3.056576	1.117155	0.219088
22	1	0.306229	-3.636393	1.896866	0.524689
23	1	0.486429	-1.829386	1.274825	0.119160
24	7	0.152414	-3.790417	0.101210	0.034082
25	8	-0.395880	-3.200930	-0.983808	-0.346522
26	1	0.454994	-2.120986	-0.956997	-0.499178
27	1	-0.101038	0.351911	3.164093	-1.702923

TSIII/IV

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	13	0.995069	-0.491381	-0.083088	0.017646
2	8	-0.766571	0.243642	1.568711	0.399953
3	8	-0.769917	0.958173	-0.729571	-0.909892
4	8	-0.653486	-1.852381	0.191193	-0.983810
5	8	-0.650200	-0.689395	-1.037302	1.424831
6	14	0.704373	-0.543686	3.022663	0.762207
7	14	0.706370	1.373656	-2.312696	-1.340319
8	14	0.659569	-3.168430	0.038831	-1.940356
9	14	0.660138	-1.197688	-1.723085	2.817498
10	1	0.466626	1.347479	1.575694	-0.024107
11	1	-0.097308	-0.881377	3.754564	-0.481196
12	1	-0.095395	-1.771698	2.697683	1.521367
13	1	-0.099625	0.379941	3.836984	1.587089
14	1	-0.098965	2.210679	-2.248814	-2.559981
15	1	-0.101908	2.112984	-2.983888	-0.246588
16	1	-0.103269	0.111504	-3.038957	-1.615088
17	1	-0.128612	-3.759260	1.376530	-2.223154
18	1	-0.130783	-2.817471	-0.590678	-3.245078
19	1	-0.126794	-4.219899	-0.799542	-1.299154
20	1	-0.126177	-2.559179	-2.310482	2.674840
21	1	-0.128531	-0.270030	-2.814164	3.227345
22	1	-0.132148	-1.245074	-0.725935	3.924845
23	7	-0.253409	4.042988	-0.004485	-0.092380
24	7	0.065248	3.466793	1.059245	0.159463
25	8	-0.540473	2.343125	1.195043	-0.649810
26	1	0.279279	4.863877	-0.017070	0.528871
27	1	0.466900	1.797756	0.120321	-0.905575

TSV/VI

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	13	0.990278	-0.477034	-0.014505	0.071377
2	8	-0.784704	0.433026	1.554190	-0.139379
3	8	-0.781262	0.865257	-1.209367	-0.211191
4	8	-0.659821	-1.662089	-0.155011	-1.172382
5	8	-0.639893	-1.039406	-0.139746	1.695151
6	14	0.693633	-0.175360	3.065100	-0.494889
7	1	-0.114105	-0.341725	3.256236	-1.959391
8	1	-0.107494	-1.481754	3.281955	0.175526
9	14	0.692736	0.756571	-2.818180	-0.625067
10	1	-0.116649	0.702358	-2.999270	-2.100035
11	1	-0.127254	1.974976	-3.510736	-0.121081
12	1	-0.109604	-0.443906	-3.446487	-0.017309
13	14	0.651309	-3.007539	-0.344254	-2.069215
14	1	-0.131768	-4.221131	-0.562218	-1.230124
15	1	-0.136924	-3.260766	0.857537	-2.916070
16	1	-0.136804	-2.882635	-1.514879	-2.985562
17	14	0.657615	-1.836895	-0.301460	3.103397
18	1	-0.131593	-3.299156	-0.514541	2.902875
19	1	-0.137527	-1.319643	-1.462117	3.886255
20	1	-0.137573	-1.675241	0.912256	3.956752
21	7	-0.300799	2.680602	0.508525	-0.068457
22	1	0.404356	2.186893	-0.473663	-0.127094
23	1	0.425547	1.867038	1.262499	-0.081147
24	7	0.128878	3.877607	0.781671	-0.000084
25	8	-0.333488	4.631745	-0.350197	-0.007155
26	1	-0.126518	0.800571	4.076977	-0.003674
27	1	0.369429	5.544973	-0.022180	0.052458

Coordinates and atomic charges for the optimized structures of all species in Fig. S1.

$Z^{-}H^{+}[NH_4NO_2]$

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	13	0.997602	0.682333	0.056847	0.260663
2	8	-0.724293	0.544183	1.797737	0.142260
3	8	-0.709808	-0.455244	-0.536890	-1.144593
4	8	-0.644063	-0.017844	-0.596895	1.679474
5	8	-0.689697	2.153769	-0.605961	-0.352906
6	14	0.678699	1.496936	3.137262	0.258857
7	1	-0.133639	0.620287	4.332179	0.420000
8	1	-0.121253	2.417993	3.072567	1.426197
9	14	0.711824	0.127834	-1.422076	-2.503373
10	1	-0.099518	-1.071110	-1.628171	-3.349535
11	1	-0.085155	1.115190	-0.574853	-3.195746
12	1	-0.085281	0.688380	-2.719407	-2.079770
13	14	0.662624	-0.502693	-1.392124	3.020162
14	1	-0.130373	-1.849753	-0.921674	3.449308
15	1	-0.130453	-0.591257	-2.860151	2.778817
16	1	-0.129635	0.441179	-1.172290	4.151767
17	14	0.667563	3.711635	-1.101433	-0.242675
18	1	-0.125899	3.920566	-2.028613	0.904595
19	1	-0.131884	4.097449	-1.818793	-1.489854
20	1	-0.128651	4.641226	0.050956	-0.072260
21	7	-0.800990	-2.262737	2.222476	-0.660665
22	1	0.278807	-2.249698	2.422059	-1.659116
23	1	0.285713	-2.614266	3.060293	-0.199679
24	1	0.349396	-1.284575	2.100751	-0.360851
25	8	-0.382238	-4.095633	0.506555	-0.028163
26	7	0.305116	-4.016111	-0.780830	-0.239018
27	8	-0.378610	-2.946085	-1.191550	-0.679340
28	1	0.417452	-1.425196	-0.663596	-0.928346
29	1	-0.124332	2.315327	3.340387	-0.969032
30	1	0.400974	-3.227275	1.091043	-0.312779

$Z^{-}H^{+}[NH_2NO+H_2O]$

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	13	1.029672	0.451432	0.126017	0.119055
2	8	-0.724204	0.829807	-0.226929	1.785949
3	8	-0.724144	-0.606795	-1.278302	-0.520843
4	8	-0.676226	1.803197	0.058782	-0.946954
5	8	-0.742066	-0.615101	1.509419	-0.086484
6	14	0.681260	2.126504	-0.470297	2.774403
7	14	0.708330	-0.034743	-2.608809	-1.438117
8	14	0.652645	3.175554	0.365799	-1.778185
9	14	0.692160	-0.404536	3.097674	-0.492785
10	1	0.448480	-1.636521	-1.171578	-0.477386
11	1	-0.125482	1.661424	-0.465298	4.188357
12	1	-0.126586	2.783767	-1.780565	2.509985
13	1	-0.125989	3.149732	0.600305	2.617311
14	1	-0.088075	-1.099055	-3.633908	-1.376270
15	1	-0.094163	0.206947	-2.193708	-2.836521
16	1	-0.089409	1.206032	-3.084579	-0.795781
17	1	-0.133085	3.296451	-0.562192	-2.937613
18	1	-0.131003	3.195591	1.759732	-2.306020
19	1	-0.128121	4.384395	0.187428	-0.925314
20	1	-0.115551	-0.035376	3.267548	-1.923299
21	1	-0.140252	-1.699322	3.802627	-0.264502
22	1	-0.119542	0.637043	3.750815	0.345034
23	1	0.347465	-0.940367	-0.624110	2.326565
24	1	0.299476	-2.203118	0.075546	2.820771
25	1	0.366281	-2.381141	1.025711	0.016736
26	7	0.165941	-3.932935	-0.257748	-0.447019
27	8	-0.417464	-3.134641	-1.190468	-0.658695
28	7	-0.354773	-3.402343	0.874445	-0.092259
29	8	-0.637538	-1.908604	-0.610600	2.209481
30	1	0.301962	-4.069970	1.614753	0.071114

TS_Z^{-}H^{+}[NH_4NO_2]- Z^{-}H^{+}[NH_2NO+H_2O]

Center Number	Atomic Number	Atomic Charges	Coordinates (Angstroms) X	Y	Z
1	13	1.014669	-0.538166	0.196720	0.116593
2	8	-0.700054	0.354113	1.609215	-0.310433
3	8	-0.687491	-0.043832	-1.041997	-1.242741
4	8	-0.687013	-2.241779	0.145206	-0.124206
5	8	-0.725433	0.083870	-0.594435	1.546391
6	14	0.667610	0.575030	3.232570	-0.170083
7	14	0.715923	-1.106280	-1.815682	-2.355976
8	14	0.662274	-3.803783	0.623113	0.011660
9	14	0.684347	-0.500013	-1.368858	2.881135
10	1	0.407535	0.903098	-1.318994	-1.204646
11	1	-0.120127	1.313324	3.742381	-1.355913
12	1	-0.127638	-0.727995	3.951846	-0.086535
13	1	-0.125704	1.359313	3.569108	1.049812
14	1	-0.094328	-0.214830	-2.638444	-3.205113
15	1	-0.082399	-2.055841	-2.663910	-1.611153
16	1	-0.080392	-1.786009	-0.772530	-3.144719
17	1	-0.131233	-4.650601	-0.165142	-0.926471
18	1	-0.126539	-4.320398	0.403233	1.391394
19	1	-0.124088	-3.971941	2.065721	-0.317115
20	1	-0.127320	-1.325368	-2.554633	2.517463
21	1	-0.130882	0.656870	-1.845837	3.689716
22	1	-0.121057	-1.326644	-0.470324	3.731456
23	1	0.316499	2.576109	1.093115	-1.134774
24	1	0.397842	3.203677	0.612613	0.530350
25	1	0.333866	2.080246	-0.623225	1.391969
26	7	0.202905	3.488053	-0.995778	-0.433510
27	8	-0.286238	2.584876	-1.562604	-0.972789
28	7	-0.601824	3.045733	-0.378080	1.135853
29	8	-0.611831	3.449863	0.943016	-0.731511
30	1	0.288120	3.740406	-0.708529	1.800181