

Supporting information

Strong external electric fields reduce explosive sensitivity. A theoretical investigation into the reaction selectivity in $\text{NH}_2\text{NO}_2\cdots\text{NH}_3$

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Figure S1 $\text{NH}_2\text{NO}_2\cdots\text{NH}_3$, in which NH_3 is only as a H-bonded donor.

Figure S2 Changes of the activation distances versus field strengths in the different field orientations for transition states at the MP2/6-311++G(2d,p) level.

Figure S3 The research scheme for the effects of external electric fields on the initiation reactions in $\text{NH}_2\text{NO}_2\cdots\text{NH}_3$.

Cartesian coordinates for the optimized geometries of reactant and transition states in the different external field strengths and orientations as well as in the absence of field.

Table S1 Barriers (E_a) and bond dissociation energies (BDE) at the MP2/6-311++G(2d,p) and CCSD(T)/6-311++G(2d,p)//MP2/6-311++G(2d,p) levels.

Field	$E_{a,TS1}(MP2)$	$E_{a,TS1}(CCSD(T))$	$E_{a,TS2}(MP2)$	$E_{a,TS2}(CCSD(T))$	BDE(MP2)	BDE(CCSD(T))
No field	68.38	77.16	176.15	190.25	257.63	239.12
z -0.010	71.29	79.26	235.4	246.18	252.05	236.75
z -0.008	75.04	81.14	219.18	237.22	253.89	227.01
z -0.006	67.02	76.55	210.22	233.12	255.72	238.46
z -0.004	69.18	79.13	190.18	208.51	256.18	238.85
z -0.002	70.22	78.27	181.23	200.17	257.54	239.07
z +0.002	71.08	79.15	176.51	191.32	258.19	241.5
z +0.004	68.99	78.53	172.18	186.57	258.42	243.64
z +0.006	72.17	79.26	170.66	185.03	259.76	245.57
z +0.008	70.02	81.18	156.03	172.31	261.22	247.16
z +0.010	74.18	85.62	158.94	177.22	262.18	248.64
y -0.010	86.55	95.17	195.62	212.31	247.92	235.32
y -0.008	81.22	94.02	194.28	213.58	249.58	238.45
y -0.006	73.17	85.18	192.1	212.12	250.61	240.42
y -0.004	70.89	82.03	187.18	208.53	253.26	238.94
y -0.002	74.25	82.96	183.25	192.54	255.2	239.13
y +0.002	73.17	83.27	181.16	190.62	259.18	242.01
y +0.004	74.22	85.18	184.23	195.18	262.25	244.72
y +0.006	75.89	87.22	190.55	209.32	265.37	246.84
y +0.008	79.03	91.05	202.58	219.18	267.85	248.89
y +0.010	87.92	98.28	214.56	228.17	269.3	259.29
x +0.010	45.89	57.03	168.51	181.55		
x +0.008			169.51	181.17		
x +0.006			170.22	182.18		
x +0.004	48.02	60.18	175.36	186.05	256.03	236.36
x +0.002	50.40	60.13	174.01	188.51	256.92	239.25
x -0.002	86.41	97.14	178.4	193.06	258.5	239.25
x -0.004	100.98	116.55	179.28	194.22	261.26	242.42
x -0.006	114.02	132.23	182.03	196.53	262.74	246.98
x -0.008	143.49	161.53	183.28	195.89	267.91	250.69
x -0.010	183.98	206.28	190.18	203.24	270.18	255.38
x -0.012	202.17	207.16	205.14	218.19		
x -0.014	239.18	257.18	212.57	230.17		
x -0.016	253.22	279.06	229.32	245.18		
x -0.018	262.17	284.18	234.18	249.55		
x -0.019	275.10	288.62	242.07	256.18		
x -0.020	291.35	296.52	257.09	272.18		

Table S2 The optimized geometrical parameters in the different field strengths and orientations at the MP2/6-311++G(2d,p) level.

Field	TS1						TS2					
	R _{O8...H7}	R _{H7...N6}	R _{N6...H5}	R _{H5...N1}	R _{N1...H4}	R _{H4...O3}	R _{O8...H7}	R _{H7...N6}	R _{N6...H5}	R _{H5...N1}	R _{N1...H4}	R _{H4...O3}
Nofield	1.607	1.073	1.100	1.580	1.019	2.260	2.700	1.018	1.905	1.040	1.291	1.320
z-0.010	1.483	1.128	1.137	1.523	1.018	2.247	2.244	1.020	2.129	1.030	1.288	1.314
z-0.008	1.528	1.113	1.131	1.530	1.019	2.250	2.262	1.020	2.078	1.032	1.286	1.318
z-0.006	1.553	1.099	1.123	1.545	1.017	2.255	2.307	1.020	2.033	1.033	1.285	1.320
z-0.004	1.572	1.085	1.115	1.562	1.019	2.256	2.376	1.019	1.987	1.035	1.283	1.324
z-0.002	1.591	1.077	1.108	1.573	1.019	2.258	2.491	1.018	1.945	1.038	1.287	1.322
z+0.002	1.613	1.072	1.096	1.582	1.019	2.263	3.200	1.017	1.872	1.044	1.294	1.316
z+0.004	1.627	1.067	1.088	1.588	1.018	2.265	4.019	1.016	1.872	1.045	1.298	1.310
z+0.006	1.650	1.060	1.080	1.596	1.020	2.266	3.805	1.016	1.842	1.050	1.300	1.310
z+0.008	1.658	1.057	1.075	1.600	1.020	2.269	3.948	1.016	1.827	1.054	1.304	1.307
z+0.01	1.688	1.055	1.061	1.612	1.019	2.272	4.534	1.017	1.829	1.055	1.312	1.300
y-0.010	1.681	1.060	1.072	1.618	1.021	2.245	2.735	1.016	1.907	1.043	1.297	1.315
y-0.008	1.667	1.066	1.081	1.613	1.019	2.247	2.722	1.016	1.909	1.042	1.294	1.318
y-0.006	1.640	1.068	1.090	1.600	1.019	2.252	2.713	1.016	1.908	1.042	1.293	1.318
y-0.004	1.622	1.072	1.095	1.587	1.020	2.256	2.708	1.018	1.908	1.041	1.293	1.319
y-0.002	1.610	1.072	1.097	1.583	1.019	2.260	2.703	1.018	1.906	1.040	1.292	1.320
y+0.002	1.608	1.070	1.098	1.581	1.019	2.257	2.711	1.017	1.906	1.040	1.292	1.320
y+0.004	1.626	1.068	1.092	1.592	1.018	2.256	2.713	1.018	1.907	1.041	1.293	1.318
y+0.006	1.640	1.063	1.083	1.598	1.019	2.254	2.719	1.019	1.909	1.041	1.294	1.317
y+0.008	1.658	1.061	1.072	1.610	1.020	2.254	2.725	1.017	1.912	1.043	1.295	1.315
y+0.010	1.672	1.058	1.068	1.616	1.020	2.253	2.730	1.017	1.915	1.044	1.297	1.314
x+0.010	1.715	1.052	1.071	1.635	1.018	2.221	2.218	1.016	2.075	1.025	1.307	1.326
x+0.008	1.712	1.055	1.080	1.629	1.017	2.223	2.239	1.018	2.068	1.030	1.300	1.327
x+0.006	1.714	1.052	1.083	1.625	1.018	2.236	2.327	1.017	2.005	1.033	1.299	1.323
x+0.004	1.716	1.053	1.092	1.613	1.018	2.244	2.458	1.017	1.988	1.035	1.295	1.323
x+0.002	1.658	1.062	1.095	1.598	1.018	2.252	2.534	1.018	1.943	1.037	1.293	1.322
x-0.002	1.562	1.084	1.106	1.559	1.019	2.268	3.017	1.018	1.874	1.044	1.290	1.317
x-0.004	1.521	1.097	1.114	1.534	1.019	2.278	3.314	1.018	1.853	1.047	1.289	1.313
x-0.006	1.481	1.111	1.124	1.507	1.020	2.288	2.940	1.018	1.833	1.053	1.286	1.313
x-0.008	1.443	1.127	1.137	1.476	1.020	2.300	2.956	1.019	1.809	1.058	1.284	1.311
x-0.010	1.467	1.117	1.100	1.606	1.026	2.303	2.955	1.019	1.785	1.064	1.283	1.310
x-0.012	1.563	1.089	1.076	1.727	1.028	2.300	2.956	1.020	1.756	1.072	1.282	1.308
x-0.014	1.402	1.102	1.058	1.652	1.029	2.322	2.949	1.020	1.725	1.081	1.281	1.306
x-0.016	1.331	1.145	1.128	1.418	1.027	2.350	2.932	1.021	1.687	1.092	1.281	1.304
x-0.018	1.256	1.258	1.253	1.382	1.025	2.368	2.904	1.021	1.637	1.110	1.282	1.302
x-0.019	1.620	1.283	1.280	1.300	1.025	2.371	2.882	1.022	1.600	1.125	1.283	1.302
x-0.020	1.187	1.315	1.315	1.255	1.024	2.382	2.835	1.022	1.535	1.154	1.286	1.299

Table S3. Transition states imaginary frequencies ($\text{Im}\nu$, cm^{-1}), Gibbs energies (ΔG , kJ/mol), reaction rate constants (k , s^{-1}), Wigner tunneling corrections (κ) in the absence and presence of fields of varying strengths and directions for the intermolecular hydrogen exchange path (TS1) at the MP2/6-311++G(2d,p) level

Field	$\text{Im}\nu$	$\Delta G_{298.15}$	$k_{298.15\text{ K}}$	$k_{298.15\text{ K}}$	$\Delta G_{688\text{ K}}$	$k_{688\text{ K}}$	$k_{688\text{ K}}$
No field	368.4	70.58	2.86×10^0	1.132	88.62	2.68×10^6	1.025
z-0.010	915.8	73.52	8.73×10^{-1}	1.815	92.55	1.35×10^6	1.153
z-0.008	872.7	77.39	1.83×10^{-1}	1.740	93.10	1.22×10^6	1.139
z-0.006	492.0	68.13	7.68×10^0	1.235	85.62	4.53×10^6	1.044
z-0.004	379.3	71.55	1.93×10^0	1.140	84.18	5.82×10^6	1.026
z-0.002	378.1	72.08	1.56×10^0	1.139	86.03	4.21×10^6	1.026
z+0.002	355.6	73.02	1.07×10^0	1.123	88.92	2.54×10^6	1.023
z+0.004	320.8	71.83	1.73×10^0	1.100	90.41	1.96×10^6	1.019
z+0.006	337.0	74.03	7.11×10^{-1}	1.110	92.50	1.36×10^6	1.021
z+0.008	293.5	72.59	1.27×10^0	1.084	87.37	3.33×10^6	1.016
z+0.010	271.9	76.27	2.88×10^{-1}	1.072	95.52	8.02×10^5	1.013
y-0.010	350.6	86.55	4.56×10^{-3}	1.119	110.38	5.97×10^4	1.022
y-0.008	327.9	83.18	1.77×10^{-2}	1.104	106.26	1.23×10^5	1.020
y-0.006	342.8	76.18	2.99×10^{-1}	1.114	95.01	8.76×10^5	1.021
y-0.004	360.7	73.18	1.00×10^0	1.126	89.17	2.43×10^6	1.024
y-0.002	367.6	76.92	2.22×10^{-1}	1.131	92.35	1.40×10^6	1.025
y+0.002	335.1	75.00	4.81×10^{-1}	1.109	93.25	1.19×10^6	1.020
y+0.004	320.7	76.24	2.92×10^{-1}	1.100	95.18	8.51×10^5	1.019
y+0.006	303.5	78.24	1.30×10^{-1}	1.090	91.00	1.77×10^6	1.017
y+0.008	349.2	82.66	2.19×10^{-2}	1.118	106.36	1.20×10^5	1.022
y+0.010	341.8	90.03	1.12×10^{-3}	1.114	108.27	8.63×10^4	1.021
x+0.010	262.0	48.04	2.54×10^4	1.067	62.18	2.72×10^8	1.013
x+0.004	260.0	50.17	1.08×10^4	1.066	60.54	3.63×10^8	1.012
x+0.002	310.4	52.99	3.45×10^3	1.094	62.15	2.74×10^8	1.018
x-0.002	445.0	88.37	2.19×10^{-3}	1.192	112.26	4.30×10^4	1.036
x-0.004	547.3	103.71	4.49×10^{-6}	1.291	128.71	2.42×10^3	1.055
x-0.006	689.6	115.53	3.82×10^{-8}	1.462	138.53	4.35×10^2	1.087
x-0.008	868.6	143.57	4.67×10^{-13}	1.733	180.02	3.08×10^{-1}	1.138
x-0.010	649.2	183.67	4.41×10^{-20}	1.410	227.18	8.08×10^{-5}	1.077
x-0.012	420.2	199.01	9.05×10^{-23}	1.172	248.26	2.03×10^{-6}	1.032
x-0.014	1124.3	236.28	2.68×10^{-29}	2.228	288.33	1.84×10^{-9}	1.231
x-0.016	1157.9	246.19	2.91×10^{-31}	2.303	336.05	4.38×10^{-13}	1.245
x-0.018	1528.7	255.11	1.34×10^{-32}	3.271	340.29	2.09×10^{-13}	1.426
x-0.019	1633.0	263.62	4.34×10^{-34}	3.591	365.03	2.76×10^{-15}	1.487
x-0.020	1638.5	278.33	1.15×10^{-36}	3.609	368.81	1.43×10^{-15}	1.490

Table S4 Mulliken charges and APT charges (in bold) of the atoms as well as the index of imaginary vibration ($\overline{A_{H7}}$ and $\overline{A_{H5}}$) of TS1 under the $-x$ -direction field at the MP2/6-311++G(2d,p) level.

	0.000	-0.002	-0.004	-0.006	-0.008	-0.010	-0.012	-0.014	-0.016	-0.018	-0.019	-0.020
O8	-0.444	-0.448	-0.452	-0.455	-0.457	-0.463	-0.474	-0.460	-0.452	-0.443	-0.439	-0.430
	-0.901	-0.916	-0.928	-0.938	-0.946	-0.936	-0.933	-0.928	-0.927	-0.923	-0.920	-0.918
H7	0.495	0.512	0.528	0.545	0.561	0.525	0.474	0.468	0.499	0.613	0.630	0.634
	0.523	0.549	0.573	0.596	0.618	0.574	0.511	0.503	0.540	0.625	0.667	0.679
N6	-0.786	-0.813	-0.840	-0.872	-0.907	-0.818	-0.718	-0.922	-1.023	-1.078	-1.145	-1.195
	-0.600	-0.628	-0.657	-0.689	-0.721	-0.646	-0.543	-0.629	-0.638	-0.754	-0.913	-0.922
H5	0.546	0.551	0.558	0.566	0.576	0.494	0.447	0.498	0.516	0.606	0.617	0.620
	0.589	0.601	0.615	0.632	0.651	0.571	0.497	0.575	0.577	0.682	0.753	0.764
N1	-0.656	-0.655	-0.654	-0.655	-0.656	-0.645	-0.693	-0.683	-0.652	-0.654	-0.612	-0.610
	-0.849	-0.846	-0.844	-0.843	-0.843	-0.768	-0.746	-0.775	-0.783	-0.825	-0.799	-0.838
$\overline{A_{H7}}$	0.352	0.356	0.358	0.365	0.375	0.395	0.364	0.360	0.352	0.367	0.368	0.371
$\overline{A_{H5}}$	0.355	0.376	0.399	0.412	0.421	0.371	0.357	0.353	0.340	0.421	0.430	0.433

Table S5 Mulliken charges and APT charges (in bold) of the atoms of TS2 under the $-x$ -direction field at the MP2/6-311++G(2d,p) level.

	0.000	-0.002	-0.004	-0.006	-0.008	-0.010	-0.012	-0.014	-0.016	-0.018	-0.019	-0.020
O3	-0.306	-0.321	-0.340	-0.341	-0.351	-0.361	-0.371	-0.381	-0.391	-0.401	-0.406	-0.409
	-0.751	-0.771	-0.790	-0.798	-0.813	-0.828	-0.844	-0.861	-0.880	-0.901	-0.914	-0.930
H4	0.425	0.421	0.418	0.411	0.405	0.400	0.394	0.388	0.382	0.375	0.371	0.365
	0.477	0.479	0.480	0.482	0.484	0.485	0.487	0.489	0.491	0.493	0.494	0.495
N1	-0.527	-0.576	-0.620	-0.565	-0.570	-0.574	-0.579	-0.584	-0.590	-0.599	-0.606	-0.619
	-0.796	-0.821	-0.838	-0.837	-0.848	-0.860	-0.874	-0.887	-0.903	-0.923	-0.935	-0.953

Table S6. Imaginary frequencies ($\text{Im}\nu$, cm^{-1}), Gibbs energies (ΔG , kJ/mol), reaction rate constants (k , s^{-1}) and corrected reaction rate constants ($k_{298.15 \text{ K,C}}$ and $k_{688 \text{ K,C}}$, s^{-1}), Wigner tunneling corrections (κ) in the absence and presence of fields of varying strengths and directions for the 1,3-intramolecular hydrogen transference path (TS2) at the MP2/6-311++G(2d,p) level.

Field	$\text{Im}\nu$	$\Delta G_{298.15}$	$k_{298.15 \text{ K}}$	$\kappa_{298.15 \text{ K}}$	$\Delta G_{688 \text{ K}}$	$k_{688 \text{ K}}$	$\kappa_{688 \text{ K}}$
No field	1955.0	158.93	9.51×10^{-16}	4.714	179.59	3.32×10^{-1}	1.697
z-0.010	1984.7	222.84	6.05×10^{-27}	4.828	252.80	9.17×10^{-7}	1.719
z-0.008	1977.6	201.03	4.01×10^{-23}	4.800	221.13	2.33×10^{-4}	1.714
z-0.006	1970.0	188.51	6.26×10^{-21}	4.771	210.02	1.63×10^{-3}	1.708
z-0.004	1960.6	172.80	3.54×10^{-18}	4.735	198.26	1.27×10^{-2}	1.701
z-0.002	1958.1	160.25	5.59×10^{-16}	4.726	182.08	2.15×10^{-1}	1.700
z+0.002	1949.4	157.28	1.85×10^{-15}	4.693	176.73	5.47×10^{-1}	1.693
z+0.004	1947.6	153.19	9.64×10^{-15}	4.686	174.10	8.66×10^{-1}	1.692
z+0.006	1939.8	152.83	1.11×10^{-14}	4.656	170.70	1.57×10^0	1.687
z+0.008	1934.2	146.05	1.72×10^{-13}	4.635	169.04	2.10×10^0	1.683
z+0.010	1927.1	142.64	6.79×10^{-13}	4.609	163.18	5.84×10^0	1.678
y-0.010	1972.0	177.92	4.48×10^{-19}	4.779	202.05	6.54×10^{-3}	1.710
y-0.008	1970.3	173.51	2.66×10^{-18}	4.772	195.07	2.22×10^{-2}	1.708
y-0.006	1962.9	170.22	1.00×10^{-17}	4.744	194.35	2.51×10^{-2}	1.703
y-0.004	1958.3	166.57	4.36×10^{-17}	4.726	186.22	1.04×10^{-1}	1.700
y-0.002	1957.2	161.39	3.53×10^{-16}	4.722	183.37	1.71×10^{-1}	1.699
y+0.002	1958.9	160.26	5.56×10^{-16}	4.729	180.09	3.04×10^{-1}	1.700
y+0.004	1959.8	163.55	1.48×10^{-16}	4.732	186.81	9.39×10^{-2}	1.701
y+0.006	1960.2	172.89	3.41×10^{-18}	4.734	196.37	1.77×10^{-2}	1.701
y+0.008	1969.4	180.62	1.51×10^{-19}	4.769	205.10	3.84×10^{-3}	1.708
y+0.010	1974.0	193.18	9.51×10^{-22}	4.786	223.29	1.59×10^{-4}	1.711
x+0.010	1985.2	149.23	4.76×10^{-14}	4.829	165.63	3.81×10^0	1.719
x+0.008	1979.4	154.44	5.82×10^{-15}	4.807	173.52	9.59×10^{-1}	1.715
x+0.006	1973.6	154.92	4.8×10^{-15}	4.785	176.06	6.15×10^{-1}	1.711
x+0.004	1968.1	156.39	2.65×10^{-15}	4.764	177.72	4.60×10^{-1}	1.707
x+0.002	1961.5	157.08	2.01×10^{-15}	4.739	178.50	4.01×10^{-1}	1.702
x-0.002	1947.4	160.77	4.53×10^{-16}	4.685	180.67	2.75×10^{-1}	1.692
x-0.004	1939.5	162.53	2.23×10^{-16}	4.655	184.66	1.37×10^{-1}	1.686
x-0.006	1927.1	167.62	2.86×10^{-17}	4.609	188.41	7.10×10^{-2}	1.678
x-0.008	1917.0	169.78	1.20×10^{-17}	4.571	193.85	2.74×10^{-2}	1.671
x-0.010	1906.4	173.2	3.01×10^{-18}	4.531	196.72	1.66×10^{-2}	1.663
x-0.012	1895.5	183.20	5.33×10^{-20}	4.491	210.02	1.63×10^{-3}	1.656
x-0.014	1884.1	190.13	3.25×10^{-21}	4.449	216.85	4.92×10^{-4}	1.648
x-0.016	1871.8	206.82	3.88×10^{-24}	4.404	239.71	9.05×10^{-6}	1.639
x-0.018	1858.7	212.95	3.27×10^{-25}	4.357	241.63	6.46×10^{-6}	1.630
x-0.019	1851.0	220.76	2.48×10^{-28}	4.329	246.46	2.78×10^{-6}	1.625
x-0.020	1843.8	233.57	7.98×10^{-29}	4.303	248.93	1.80×10^{-6}	1.620

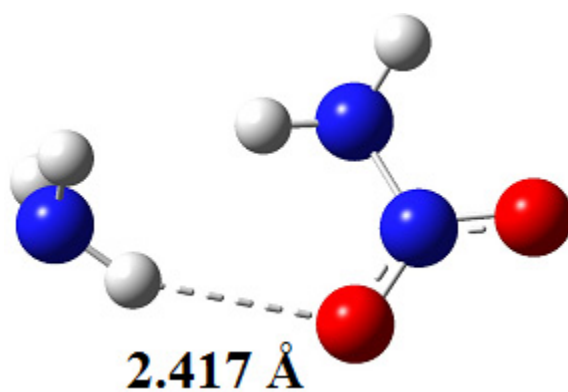
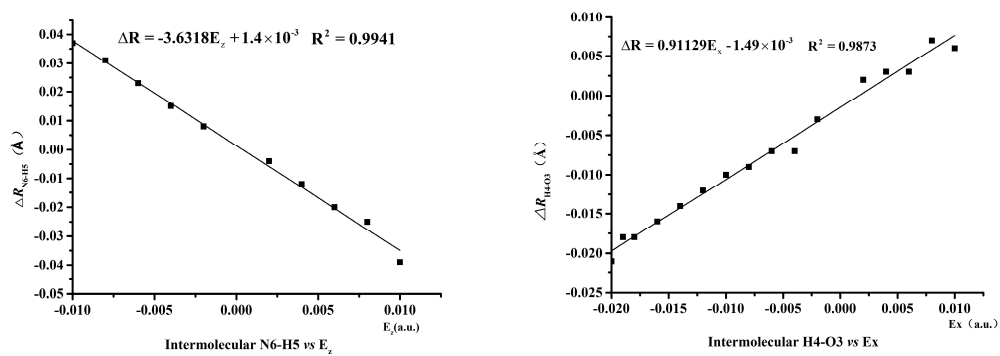


Figure S1 $\text{NH}_2\text{NO}_2 \cdots \text{NH}_3$, in which NH_3 is only as a H-bonded donor and the binding energy is 18.50 kJ/mol at the MP2/6-311++G(2d,p) level, 32.0 kJ/mol weaker than that of the $\text{NH}_2\text{NO}_2 \cdots \text{NH}_3$ in which NH_3 is not only as a H-bonded donor, but also as a H-bonded acceptor.



N6...H5 distances vs. E_z (TS1) H4...O3 distances vs. E_x (TS2)

Figure S2 Changes of the activation distances versus field strengths in the different field orientations for transition states at the MP2/6-311++G(2d,p) level.

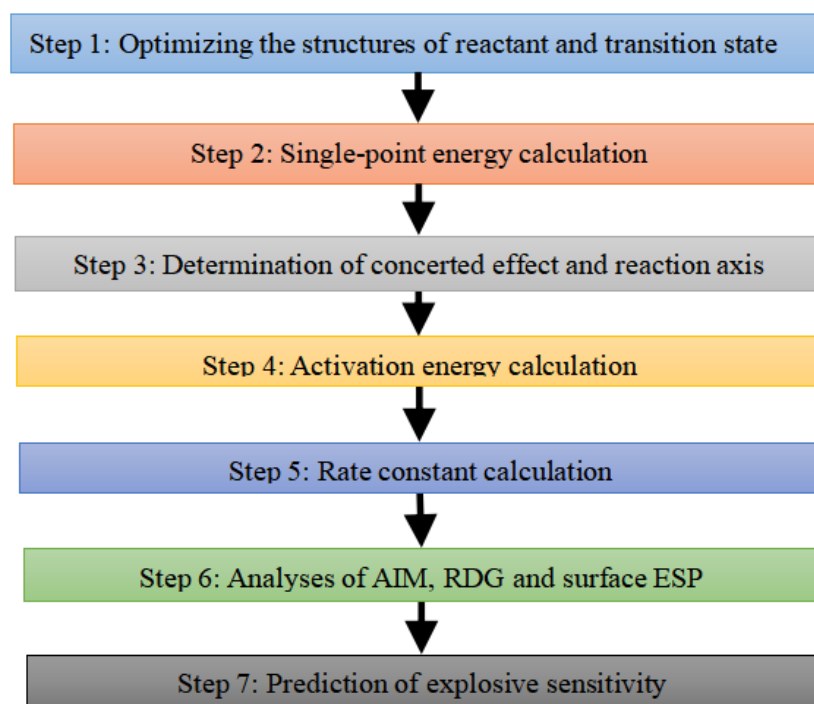


Figure S3 The research scheme for the effects of external electric fields on the initiation reactions in $\text{NH}_2\text{NO}_2\cdots\text{NH}_3$

Cartesian coordinates for the optimized geometries of reactant and transition states

TS1:

No field

Reactant

N,0,-0.1388307297,0.3519007669,-0.0298998831
N,0,-0.158585254,0.0031223882,1.3038966994
O,0,-1.236844475,-0.3528205867,1.7772334304
O,0,0.900358496,0.131879902,1.9225315384
N,0,2.7033834144,-0.043980718,-0.6781055687
H,0,2.889801177,0.0147217715,0.3203031404
H,0,3.1127304258,-0.9110755331,-1.0118374402
H,0,3.2094764427,0.7148728084,-1.1243657356
H,0,0.8028090931,0.1957712203,-0.4242245001
H,0,-0.9164652703,-0.0993088494,-0.497773551

Transition state

N	-0.010478778648	-0.005312276003	-0.003318686965
N	-0.009170612835	-0.000152113714	1.320231600914
H	0.970948482051	0.001744848153	-0.276105580404
O	-1.153543040165	-0.007109522133	1.910594308023
O	1.039014554030	0.010487964201	1.982432904788
N	-2.559188570973	-0.025389807317	-0.247643245452
H	-1.498157123278	-0.017793132824	-0.535555588187
H	-2.311692572416	-0.019179830342	0.796074235024
H	-3.049754405547	-0.867900889765	-0.529332097233
H	-3.064770932932	0.805591759230	-0.536769852666

X-20:

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

N,1,B5,2,A4,3,D3,0

H,6,B6,1,A5,2,D4,0

H,6,B7,1,A6,2,D5,0

H,6,B8,1,A7,2,D6,0

H,6,B9,1,A8,2,D7,0

Variables:

B1=1.32476608

B2=1.01823686
B3=1.2819809
B4=1.24345158
B5=2.57792323
B6=1.09523203
B7=1.06236915
B8=1.0153425
B9=1.01538045
A1=105.32706857
A2=117.60384661
A3=121.86083285
A4=95.57267284
A5=20.40458392
A6=72.76626011
A7=120.8995876
A8=121.12028983
D1=-179.94544462
D2=0.05589426
D3=179.42228644
D4=-180.04147478
D5=0.32024234
D6=-105.85366849
D7=106.43835099

X+20:

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

N,1,B5,2,A4,3,D3,0

H,6,B6,1,A5,2,D4,0

H,6,B7,1,A6,2,D5,0

H,6,B8,1,A7,2,D6,0

H,6,B9,1,A8,2,D7,0

Variables:

B1=1.3221599

B2=1.01898847

B3=1.2936114

B4=1.23607688

B5=2.54459155

B6=1.1057071

B7=1.08425361

B8=1.01419313
B9=1.01416269
A1=105.69919206
A2=116.86802539
A3=122.81084474
A4=95.52378695
A5=20.60154275
A6=69.88630919
A7=120.99180704
A8=120.96648871
D1=-179.67917093
D2=0.36745183
D3=178.75000348
D4=-179.39346888
D5=0.54816095
D6=-105.09118685
D7=106.1306122

X-40:

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

N,1,B5,2,A4,3,D3,0

H,6,B6,1,A5,2,D4,0

H,6,B7,1,A6,2,D5,0

H,6,B8,1,A7,2,D6,0

H,6,B9,1,A8,2,D7,0

Variables:

B1=1.32089265

B2=1.01935414

B3=1.29927005

B4=1.23263617

B5=2.52922666

B6=1.11358831

B7=1.09657716

B8=1.01370263

B9=1.01364829

A1=105.93254452

A2=116.47458241

A3=123.28022002

A4=95.59213186

A5=20.29844094
A6=68.87702401
A7=120.89700016
A8=120.86513912
D1=-179.5199595
D2=0.53052315
D3=178.09645162
D4=-179.07037065
D5=0.85913947
D6=-104.7639165
D7=106.43050888

X+40:

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

N,1,B5,2,A4,3,D3,0

H,6,B6,1,A5,2,D4,0

H,6,B7,1,A6,2,D5,0

H,6,B8,1,A7,2,D6,0

H,6,B9,1,A8,2,D7,0

Variables:

B1=1.3258996

B2=1.01786562

B3=1.27627887

B4=1.24732872

B5=2.59723396

B6=1.0919707

B7=1.05302189

B8=1.01601254

B9=1.01603557

A1=105.21214011

A2=117.93193144

A3=121.40328805

A4=95.65202037

A5=19.85830996

A6=74.72220198

A7=120.90878928

A8=120.87399876

D1=-180.08621575

D2=-0.0936819

D3=180.003156
D4=-180.01608943
D5=0.01057999
D6=-106.73814733
D7=106.70604175

X-60

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

N,1,B5,2,A4,3,D3,0

H,6,B6,1,A5,2,D4,0

H,6,B7,1,A6,2,D5,0

H,6,B8,1,A7,2,D6,0

H,6,B9,1,A8,2,D7,0

Variables:

B1=1.31938513

B2=1.01973854

B3=1.30524575

B4=1.22912827

B5=2.5159466

B6=1.12434135

B7=1.11077024

B8=1.01325224

B9=1.01315745

A1=106.26740374

A2=116.08502387

A3=123.74684628

A4=95.64737975

A5=19.76314592

A6=67.92330165

A7=121.14673759

A8=120.28866178

D1=-179.21097559

D2=0.92390672

D3=177.34449269

D4=-177.73673267

D5=1.22891572

D6=-104.42319731

D7=107.01625147

X-80

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

N,1,B5,2,A4,3,D3,0

H,6,B6,1,A5,2,D4,0

H,6,B7,1,A6,2,D5,0

H,6,B8,1,A7,2,D6,0

H,6,B9,1,A8,2,D7,0

Variables:

B1=1.31787918

B2=1.02008827

B3=1.31100843

B4=1.22582452

B5=2.50283161

B6=1.13740938

B7=1.12683476

B8=1.01280635

B9=1.01285548

A1=106.61767273

A2=115.65535255

A3=124.24520474

A4=95.79106852

A5=19.10421865

A6=67.11703471

A7=120.82884635

A8=120.23606372

D1=-179.70982094

D2=0.35900574

D3=178.83263439

D4=-178.93777366

D5=0.65123997

D6=-105.30066451

D7=106.66529611

X-100

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0
N,1,B5,2,A4,3,D3,0
H,6,B6,1,A5,2,D4,0
H,6,B7,1,A6,2,D5,0
H,6,B8,1,A7,2,D6,0
H,6,B9,1,A8,2,D7,0

Variables:

B1=1.32423099
B2=1.02560161
B3=1.31459974
B4=1.22902223
B5=2.57678925
B6=1.09953595
B7=1.11658817
B8=1.01563818
B9=1.01180116
A1=104.33472374
A2=114.83924737
A3=124.90113353
A4=85.71997612
A5=21.56375557
A6=68.17713432
A7=114.85309395
A8=126.2302801
D1=-162.2961559
D2=18.03809513
D3=120.7864902
D4=-168.79860112
D5=25.286796
D6=-81.75266927
D7=131.1747262

X-120

Z-Matrix found in file.

N

N,1,B1
H,1,B2,2,A1
O,2,B3,1,A2,3,D1,0
O,2,B4,1,A3,3,D2,0
N,1,B5,2,A4,3,D3,0
H,6,B6,1,A5,2,D4,0
H,6,B7,1,A6,2,D5,0
H,6,B8,1,A7,2,D6,0
H,6,B9,1,A8,2,D7,0

Variables:

B1=1.32471097
B2=1.02681613
B3=1.31521818
B4=1.23054739
B5=2.60322289
B6=1.08854952
B7=1.10674758
B8=1.01684948
B9=1.01189274
A1=104.02423173
A2=114.71770185
A3=124.98728868
A4=82.56572963
A5=22.87282952
A6=69.01421569
A7=112.36354585
A8=128.92967158
D1=-160.03266011
D2=19.6423121
D3=112.08846437
D4=-171.06441625
D5=28.28533239
D6=-79.05739406
D7=134.30757294

X-160

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

N,1,B5,2,A4,3,D3,0

H,6,B6,1,A5,2,D4,0

H,6,B7,1,A6,2,D5,0

H,6,B8,1,A7,2,D6,0

H,6,B9,1,A8,2,D7,0

Variables:

B1=1.32495867
B2=1.02771923
B3=1.31247411
B4=1.23422498
B5=2.64288296

B6=1.0758513
B7=1.08877286
B8=1.01852699
B9=1.01241144
A1=103.72248542
A2=114.86630281
A3=124.81460031
A4=78.24164226
A5=24.77403931
A6=70.75212768
A7=109.04771801
A8=132.52878978
D1=-158.54563483
D2=19.80758798
D3=102.55917696
D4=-174.59209227
D5=31.12648066
D6=-76.57005184
D7=137.61589147

X-180

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

N,1,B5,2,A4,3,D3,0

H,6,B6,1,A5,2,D4,0

H,6,B7,1,A6,2,D5,0

H,6,B8,1,A7,2,D6,0

H,6,B9,1,A8,2,D7,0

Variables:

B1=1.32505944

B2=1.02775956

B3=1.31261747

B4=1.23413274

B5=2.64461625

B6=1.07609464

B7=1.0888029

B8=1.01854396

B9=1.01240596

A1=103.73933701

A2=114.8790224

A3=124.82818125
A4=78.17485935
A5=24.75185836
A6=70.71383816
A7=109.19900298
A8=132.35091181
D1=-158.46467261
D2=19.88301627
D3=102.42187811
D4=-174.29941285
D5=31.15988758
D6=-76.49966314
D7=137.6929242

X-200

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

N,1,B5,2,A4,3,D3,0

H,6,B6,1,A5,2,D4,0

H,6,B7,1,A6,2,D5,0

H,6,B8,1,A7,2,D6,0

H,6,B9,1,A8,2,D7,0

Variables:

B1=1.31006812

B2=1.02403127

B3=1.34787581

B4=1.20599937

B5=2.49894421

B6=1.31480426

B7=1.31473005

B8=1.01431839

B9=1.01327905

A1=109.18197208

A2=113.06744557

A3=127.08729458

A4=95.47029446

A5=13.1371007

A6=61.58049745

A7=117.44063716

A8=117.20337167

D1=-170.04493971
D2=12.01358154
D3=154.28672267
D4=-167.78245348
D5=11.20558146
D6=-99.09675308
D7=125.67011322

TS2:

No field

Transition state

N,0,0.179619372,-0.2283193224,0.142838143
N,0,-0.1247602028,-0.0616459716,1.4036723497
H,0,1.1816847343,-0.072717186,-0.0897998946
H,0,-1.0945383133,-0.4300438482,0.1910942552
O,0,0.5823763775,0.2237800273,2.3578368918
O,0,-1.4289611332,-0.2749630091,1.4584875998
N,0,3.0302499376,0.3217192624,0.1487372851
H,0,2.9837125782,0.4858585426,1.1518750921
H,0,3.7056675296,-0.4211926919,-0.0032235565
H,0,3.4105191947,1.1618770505,-0.2763537668

X-20

N	-0.175000568660	-0.016541795048	-0.121303108722
N	0.118752837647	0.001967870491	1.152654841187
H	0.642271936788	-0.011473379305	-0.770851623221
H	-1.321324592105	-0.033711303255	0.469256368044
O	1.198679568799	0.028431022991	1.717580278770
O	-1.061889977312	-0.014329044743	1.759945333480
N	2.335441970332	0.006860291151	-1.573143079178
H	2.933584109159	0.027279189126	-0.750232437086
H	2.577704090172	0.819960715100	-2.132099782825
H	2.605879623949	-0.810835563972	-2.111996795678

X+20

N	-0.255417503917	0.042739967437	-0.167989131395
N	0.176742864421	-0.014328874366	1.064797046536
H	0.488112377599	0.040892699953	-0.891040128648
H	-1.333103169588	0.046235067744	0.545935763050
O	1.318559784159	-0.063037212947	1.502183572173
O	-0.918017689665	-0.009060554660	1.799656970689
N	2.317266873102	-0.001699898996	-1.543543059010
H	2.719343594982	-0.042756161795	-0.609710042162

H	2.699924338864	0.816281238173	-2.007177665067
H	2.640687530018	-0.817658268400	-2.053303326327

X-40

N	-0.122022267767	-0.020532320635	-0.086900440473
N	0.083296327694	0.016158623094	1.203500206988
H	0.731457311225	-0.015076627970	-0.693805844236
H	-1.304766338867	-0.044391510199	0.423764545842
O	1.116477564479	0.061560196818	1.844886861494
O	-1.142738582089	-0.006879899737	1.726499633064
N	2.351479162371	-0.001217268330	-1.592903285662
H	3.045646098424	0.021910698423	-0.849157024277
H	2.534116292342	0.807431852079	-2.180732145009
H	2.561153429749	-0.821355743163	-2.155342517961

X+40

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

H,1,B5,2,A4,3,D3,0

N,3,B6,1,A5,2,D4,0

H,7,B7,3,A6,1,D5,0

H,7,B8,3,A7,1,D6,0

H,7,B9,3,A8,1,D7,0

Variables:

B1=1.30559576

B2=1.05970935

B3=1.34645671

B4=1.21423105

B5=1.28419035

B6=1.80300255

B7=1.01884704

B8=1.01736068

B9=1.01735739

A1=114.23302934

A2=103.59176692

A3=131.71451908

A4=75.90737622

A5=165.78795319

A6=103.47048306

A7=117.33624652

A8=117.41143768
D1=179.79853466
D2=-0.20340921
D3=-179.7534042
D4=0.00883097
D5=-0.140054
D6=115.90407972
D7=-116.22961861

X-60

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

H,1,B5,2,A4,3,D3,0

N,3,B6,1,A5,2,D4,0

H,7,B7,3,A6,1,D5,0

H,7,B8,3,A7,1,D6,0

H,7,B9,3,A8,1,D7,0

Variables:

B1=1.30625597

B2=1.05306498

B3=1.33909053

B4=1.21611493

B5=1.28591507

B6=1.8326124

B7=1.01833102

B8=1.01682101

B9=1.0168253

A1=114.55621031

A2=103.82419931

A3=131.32256192

A4=75.87202225

A5=165.21260664

A6=102.21086602

A7=117.53111488

A8=117.41928478

D1=-179.98514901

D2=0.01887718

D3=179.98380928

D4=-0.17476666

D5=0.35087429

D6=116.08789225
D7=-115.32594283

X+60

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

H,1,B5,2,A4,3,D3,0

N,3,B6,1,A5,2,D4,0

H,7,B7,3,A6,1,D5,0

H,7,B8,3,A7,1,D6,0

H,7,B9,3,A8,1,D7,0

Variables:

B1=1.30548354

B2=1.06120408

B3=1.3479788

B4=1.21388523

B5=1.28385962

B6=1.79660799

B7=1.01896273

B8=1.01746844

B9=1.01746556

A1=114.15224772

A2=103.55722912

A3=131.79040741

A4=75.92309412

A5=165.7903996

A6=103.60503243

A7=117.39774638

A8=117.40051628

D1=179.94909198

D2=-0.05906613

D3=-179.92627008

D4=-0.01669875

D5=-0.32728055

D6=115.75523073

D7=-116.4232273

X-80

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

H,1,B5,2,A4,3,D3,0

N,3,B6,1,A5,2,D4,0

H,7,B7,3,A6,1,D5,0

H,7,B8,3,A7,1,D6,0

H,7,B9,3,A8,1,D7,0

Variables:

B1=1.30573489

B2=1.05824174

B3=1.34493421

B4=1.21459516

B5=1.28448568

B6=1.8094018

B7=1.01873248

B8=1.0172448

B9=1.01724227

A1=114.310453

A2=103.63966949

A3=131.6351336

A4=75.89995459

A5=165.72386336

A6=103.24318991

A7=117.32333092

A8=117.44251153

D1=-180.17634172

D2=-0.183666

D3=180.21814725

D4=0.12632091

D5=0.04355426

D6=116.02051746

D7=-115.99137451

X+80

N	-0.321191439387	0.035105800774	-0.179647815685
---	-----------------	----------------	-----------------

N	0.210446049726	0.000075255121	1.013364615625
---	----------------	----------------	----------------

H	0.348286944664	0.032712550088	-0.962083738885
---	----------------	----------------	-----------------

H	-1.343983341803	0.037679388696	0.621818494634
---	-----------------	----------------	----------------

O	1.391855703116	-0.030606036140	1.355988437460
---	----------------	-----------------	----------------

O	-0.807916108811	0.004216828622	1.834863880928
---	-----------------	----------------	----------------

N	2.332382715280	-0.010805752166	-1.543866771648
---	----------------	-----------------	-----------------

H	2.561782593778	-0.047136768567	-0.553193558658
H	2.768797006282	0.809462124290	-1.949266387850
H	2.713638875744	-0.833095383510	-1.998167161857

X-100

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

H,1,B5,2,A4,3,D3,0

N,3,B6,1,A5,2,D4,0

H,7,B7,3,A6,1,D5,0

H,7,B8,3,A7,1,D6,0

H,7,B9,3,A8,1,D7,0

Variables:

B1=1.30518078

B2=1.06424691

B3=1.35113368

B4=1.21316037

B5=1.28332523

B6=1.7845543

B7=1.01918585

B8=1.01768789

B9=1.01768189

A1=113.99319547

A2=103.45882901

A3=131.95199757

A4=75.9298606

A5=165.93499663

A6=104.0182312

A7=117.39123898

A8=117.37810914

D1=180.66822294

D2=0.70625861

D3=-180.8391107

D4=-0.01771556

D5=-0.51607076

D6=115.68148959

D7=-116.71631899

Z-20

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

H,1,B3,2,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

O,2,B5,1,A4,3,D3,0

N,3,B6,1,A5,2,D4,0

H,7,B7,3,A6,1,D5,0

H,7,B8,3,A7,1,D6,0

H,7,B9,3,A8,1,D7,0

Variables:

B1=1.31058914

B2=1.03750833

B3=1.28739055

B4=1.22043767

B5=1.31973644

B6=1.94538703

B7=1.01838452

B8=1.01548309

B9=1.01547366

A1=114.5941322

A2=75.81857942

A3=130.38073806

A4=104.31837988

A5=154.73664805

A6=92.59798611

A7=120.29430214

A8=120.22051497

D1=-177.53232972

D2=-2.09297614

D3=177.99130625

D4=0.56447459

D5=0.86664301

D6=-110.57849399

D7=112.32642335

Z+20

N	-0.149241279946	0.009769008914	-0.101583063578
N	0.097332431603	0.001134163506	1.179861893573
H	0.687101144080	0.005019878130	-0.727018748631
H	-1.320388746495	0.017527262338	0.448015325364
O	1.157000900478	-0.011592578290	1.786865391900
O	-1.103551212668	0.009218526666	1.745671403799
N	2.353607364501	-0.006258596161	-1.578849552159

H	3.022297859288	-0.018899419974	-0.813191049218
H	2.563591191509	0.811477170368	-2.143968858896
H	2.546349348534	-0.819787413654	-2.155992738459

Z-40

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

H,1,B3,2,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

O,2,B5,1,A4,3,D3,0

N,3,B6,1,A5,2,D4,0

H,7,B7,3,A6,1,D5,0

H,7,B8,3,A7,1,D6,0

H,7,B9,3,A8,1,D7,0

Variables:

B1=1.31353042

B2=1.03489212

B3=1.28346986

B4=1.21918705

B5=1.31705149

B6=1.9872198

B7=1.01908536

B8=1.01560669

B9=1.01556251

A1=114.52352175

A2=75.89306653

A3=130.35013654

A4=104.21020309

A5=151.87748123

A6=89.69249097

A7=121.21773301

A8=121.8419305

D1=-178.20296006

D2=-1.52565847

D3=178.55238694

D4=0.24620764

D5=0.86686434

D6=-108.59278541

D7=110.48843602

Z+40

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

H,1,B3,2,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

O,2,B5,1,A4,3,D3,0

N,3,B6,1,A5,2,D4,0

H,7,B7,3,A6,1,D5,0

H,7,B8,3,A7,1,D6,0

H,7,B9,3,A8,1,D7,0

Variables:

B1=1.30265162

B2=1.0454716

B3=1.29834937

B4=1.22187094

B5=1.33023601

B6=1.87154798

B7=1.0160031

B8=1.01664784

B9=1.01664338

A1=118.64370866

A2=75.67506797

A3=130.98455221

A4=104.30211979

A5=171.83961663

A6=114.35831228

A7=111.21190537

A8=111.21528024

D1=-180.02754857

D2=0.0206345

D3=180.01884165

D4=179.93051573

D5=-180.24923403

D6=-301.0866818

D7=-59.40868389

Z-60

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

H,1,B3,2,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

O,2,B5,1,A4,3,D3,0

N,3,B6,1,A5,2,D4,0
H,7,B7,3,A6,1,D5,0
H,7,B8,3,A7,1,D6,0
H,7,B9,3,A8,1,D7,0

Variables:

B1=1.31790388
B2=1.03315189
B3=1.28508402
B4=1.21766766
B5=1.31488821
B6=2.03268641
B7=1.01962409
B8=1.01593682
B9=1.01563334
A1=113.88746263
A2=75.57243027
A3=130.33394629
A4=104.13179202
A5=149.95475099
A6=87.37517589
A7=120.87904661
A8=124.27506664
D1=-166.16326877
D2=-11.79085212
D3=168.79556408
D4=1.73121132
D5=6.3648589
D6=-101.0983475
D7=114.54740621

Z+60

N	-0.039682674490	-0.001398480124	-0.035611880527
N	0.030428490692	-0.000614414119	1.263048788730
H	0.862310461283	-0.000708510490	-0.573890833217
H	-1.280593379862	-0.002298685985	0.352640537847
O	0.992058984461	0.000744613667	2.018931084239
O	-1.242325761227	-0.001568005009	1.661652544055
N	2.395697647373	0.000607704113	-1.594733738195
H	3.249677596146	0.005042111248	-1.044039514378
H	2.440655762786	0.811710916033	-2.206570290995
H	2.445871872129	-0.813909246083	-2.201616700524

Z-80

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

H,1,B3,2,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

O,2,B5,1,A4,3,D3,0

N,3,B6,1,A5,2,D4,0

H,7,B7,3,A6,1,D5,0

H,7,B8,3,A7,1,D6,0

H,7,B9,3,A8,1,D7,0

Variables:

B1=1.32239305

B2=1.0315668

B3=1.28608256

B4=1.21612544

B5=1.31274174

B6=2.07820065

B7=1.02008936

B8=1.01640997

B9=1.01572895

A1=113.32692005

A2=75.32012988

A3=130.27717453

A4=104.06855727

A5=148.38221158

A6=85.27997368

A7=118.93559512

A8=128.11283802

D1=-161.27150648

D2=-16.07758394

D3=164.76947839

D4=0.87255942

D5=12.39371315

D6=-93.0260448

D7=119.32363154

Z+80

N	-0.007375234783	-0.001653929614	-0.019021990300
N	0.019786052556	-0.001662286246	1.279221327468
H	0.909253343992	-0.000878308414	-0.538759402561
H	-1.263639883283	0.002056657991	0.329983612864
O	0.953840522432	-0.004432582044	2.071129038268
O	-1.267544453050	0.001328559542	1.637047298085
N	2.400411313912	0.000793624077	-1.594389837859

H	3.292948832800	0.004340846515	-1.108692787618
H	2.406475218138	0.810217642390	-2.210968626235
H	2.409943287208	-0.812502220810	-2.205738632504

Z-100

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

H,1,B3,2,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

O,2,B5,1,A4,3,D3,0

N,3,B6,1,A5,2,D4,0

H,7,B7,3,A6,1,D5,0

H,7,B8,3,A7,1,D6,0

H,7,B9,3,A8,1,D7,0

Variables:

B1=1.32740138

B2=1.03012506

B3=1.28824699

B4=1.21440953

B5=1.31078732

B6=2.12881078

B7=1.01587507

B8=1.0203087

B9=1.01707661

A1=112.67279231

A2=74.98409685

A3=130.20429766

A4=104.0016595

A5=146.79150785

A6=133.84095908

A7=83.76848425

A8=114.73593505

D1=-156.73105242

D2=-20.12034391

D3=160.99319081

D4=-1.07369322

D5=127.56106659

D6=21.35990221

D7=277.5527353

Z+100

Z-Matrix found in file.

N

N,1,B1

H,1,B2,2,A1

O,2,B3,1,A2,3,D1,0

O,2,B4,1,A3,3,D2,0

H,1,B5,2,A4,3,D3,0

N,3,B6,1,A5,2,D4,0

H,7,B7,3,A6,1,D5,0

H,7,B8,3,A7,1,D6,0

H,7,B9,3,A8,1,D7,0

Variables:

B1=1.29625438

B2=1.05537491

B3=1.226162

B4=1.33811297

B5=1.31154641

B6=1.82910595

B7=1.01772662

B8=1.01681931

B9=1.01905235

A1=121.71827073

A2=131.67708891

A3=104.44123806

A4=75.42348455

A5=160.73357463

A6=113.33090382

A7=120.09910528

A8=105.62066171

D1=-0.37363752

D2=179.63092786

D3=-179.56097731

D4=-179.68805356

D5=88.41356942

D6=214.90117145

D7=-26.25129388

0 field Reactant:

N,0,0.1315512978,-0.3477164016,0.1549957505

N,0,0.2024178136,-0.0114519864,1.4903546951

H,0,0.8868602495,0.1133007097,-0.339183404

O,0,-0.8300012992,-0.153636111,2.149555932

O,0,1.2963527893,0.3475744522,1.9236516742

N,0,-2.7380492168,0.0234710704,-0.3742172461

H,0,-0.8261590755,-0.1944349912,-0.1998490218

H,0,-2.8822720489,-0.0442098805,0.6305718656
H,0,-3.2501053109,-0.7405830812,-0.8044715352
H,0,-3.173727979,0.8861289397,-0.6852553203

X-Reactant

N	0	-0.217235	0.371967	0.171327
N	0	-0.485107	-0.011050	1.466995
H	0	0.784115	0.225251	-0.050710
O	0	0.437530	0.094559	2.275816
O	0	-1.635687	-0.373764	1.720416
N	0	2.667004	-0.011395	-0.151015
H	0	2.850771	-0.007609	0.849457
H	0	3.187807	0.764555	-0.549517
H	0	3.078275	-0.861652	-0.524699
H	0	-0.893111	-0.065585	-0.443826

X+20-Reactant

N	0	-0.266916	0.339103	0.104534
N	0	-0.409452	-0.010957	1.431489
H	0	0.705060	0.187355	-0.199051
O	0	0.588181	0.124560	2.146446
O	0	-1.522726	-0.372401	1.802500
N	0	2.667228	-0.006668	-0.136463
H	0	2.612023	0.064220	0.877113
H	0	3.229234	0.770672	-0.468252
H	0	3.169403	-0.860094	-0.358585
H	0	-0.997673	-0.110513	-0.435488

X+80-Reactant

N	0	-0.209689	0.287806	-0.022178
N	0	-0.263905	0.064188	1.340375
H	0	0.685809	-0.022190	-0.401867
O	0	0.816766	0.104685	1.947001
O	0	-1.366270	-0.092037	1.842377
N	0	2.845270	-0.209657	-0.210282
H	0	2.515270	-0.085843	0.745959
H	0	3.397859	0.603734	-0.458357
H	0	3.449903	-1.023004	-0.235636
H	0	-1.051467	-0.074482	-0.458663

X-80-Reactant

N	0	-0.022465	0.341511	0.307398
N	0	-0.694528	0.036916	1.458254
H	0	0.997394	0.119490	0.336957

O	0	-1.909114	-0.198581	1.353432
O	0	-0.061973	0.076761	2.510597
N	0	2.806724	-0.228754	0.042758
H	0	3.321312	0.022633	0.884074
H	0	3.067641	-1.190445	-0.161502
H	0	3.211465	0.332006	-0.703757
H	0	-0.540553	-0.021045	-0.482950

X-160-Reactant

N	0	0.286229	-0.261650	1.100046
N	0	-0.972256	0.068280	0.813334
O	0	-1.848504	-0.152747	1.680679
O	0	-1.217058	0.538289	-0.307208
N	0	2.647016	0.495464	-0.133366
H	0	3.096367	1.299025	0.304177
H	0	3.306193	-0.271574	0.002121
H	0	2.671533	0.687990	-1.132771
H	0	1.107353	0.100445	0.509988
H	0	0.405491	-0.500253	2.076016

X-200-Reactant

N	0	0.086284	0.098858	1.048053
N	0	-1.219853	0.120614	0.906236
O	0	-1.994046	-0.060796	1.913317
O	0	-1.719556	0.323145	-0.238144
N	0	2.813398	0.319773	-0.150773
H	0	3.034573	1.260157	-0.488062
H	0	3.461776	0.103587	0.613834
H	0	2.995565	-0.342834	-0.908663
H	0	1.810955	0.259841	0.169202
H	0	0.213268	-0.079078	2.048014