Supporting information

A dynamic prediction of stability for nitromethane in external electric field

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Supplementary Tables

Table S1 Total energies of CH_3NO_2 and radicals, and the C–NO_2 bond dissociation energies in the different external electric field strengths and orientations at the CCSD/6-311++G(2d,p)//MP2/6-311++G(2d,p) level.

Table S2 Total energies of the reactants and transition states, and barriers of three decomposition paths in the different external electric field strengths and orientations at the CCSD/6-311++G(2d,p)//MP2/6-311++G(2d,p) level.

Table S3 The optimized geometrical parameters and AIM results of TS-2 in the different field strengths and orientations at the MP2/6-311++G(2d,p) level.

Table S4 part1. The optimized geometrical parameters and AIM results of TS-3 in the different field strengths and orientations at the MP2/6-311++G(2d,p) level.

Table S4 part2. The optimized geometrical parameters and AIM results of TS-3 in the different field strengths and orientations at the MP2/6-311++G(2d,p) level.

Fig. S1 Selected structures of the nitromethane dimer in the different external electric field strengths and orientations (including those in no field) at the MP2/6-311++G(2d,p) level.

Table S1 Total energies of CH_3NO_2 and radicals (E, a.u.), and the C–NO_2 bond dissociation energies (BDE, kJ/mol) in the different external electric field strengths and orientations at the CCSD/6-311++G(2d,p)//MP2/6-311++G(2d,p) level.

Field (a.u.)	E_{CH3NO2}/(a.u.)	$E_{CH3.}$/(a.u.)	$E_{NO2.}$/(a.u.)	BDE /(kJ/mol)
Z -0.010	-244.5323	-39.7158	-204.7114	275.90
Z -0.008	-244.5323	-39.7159	-204.7114	275.73
Z -0.006	-244.5323	-39.7160	-204.7114	275.56
Z -0.004	-244.5323	-39.7160	-204.7114	275.40
Z -0.002	-244.5324	-39.7161	-204.7114	275.29
Z +0.002	-244.5324	-39.7161	-204.7114	275.30
Z +0.004	-244.5324	-39.7160	-204.7114	275.41
Z +0.006	-244.5323	-39.7160	-204.7114	275.55
Z +0.008	-244.5323	-39.7159	-204.7114	275.71
Z +0.010	-244.5322	-39.7158	-204.7114	275.88
X -0.010	-244.5345	-39.7161	-204.7114	280.90
X -0.008	-244.5337	-39.7161	-204.7114	278.86
X -0.006	-244.5331	-39.7161	-204.7114	277.28
X -0.004	-244.5324	-39.7161	-204.7112	275.80
X -0.002	-244.5324	-39.7161	-204.7114	275.38
X +0.002	-244.5324	-39.7161	-204.7114	275.38
X +0.004	-244.5324	-39.7161	-204.7112	275.80
X +0.006	-244.5331	-39.7161	-204.7114	277.27
X +0.008	-244.5337	-39.7161	-204.7114	278.86
X +0.010	-244.5345	-39.7161	-204.7114	280.90
Y -0.010	-244.5323	-39.7161	-204.7114	274.97
Y -0.008	-244.5323	-39.7161	-204.7114	275.07
Y -0.006	-244.5323	-39.7161	-204.7114	275.14
Y -0.004	-244.5323	-39.7161	-204.7114	275.19
Y -0.002	-244.5324	-39.7161	-204.7114	275.23
Y +0.002	-244.5324	-39.7161	-204.7114	275.24
Y +0.004	-244.5324	-39.7161	-204.7114	275.23
Y +0.006	-244.5324	-39.7161	-204.7114	275.20
Y +0.008	-244.5323	-39.7161	-204.7114	275.15
Y +0.010	-244.5323	-39.7161	-204.7114	275.07

Table S2 Total energies of the reactants and transition states (E, a.u.), and barriers (E_a, kJ/mol) of three decomposition paths in the different external electric field strengths and orientations at the CCSD/6-311++G(2d,p)//MP2/6-311++G(2d,p) level.

Field (a.u.)	$E_{(TS-1)}$ /(a.u.)	E_{CH3NO2} /(a.u.)	$Ea_{(TS-1)}$ /(kJ/mol)	$E_{(TS-2)}$ /(a.u.)	$Ea_{(TS-2)}$ /(kJ/mol)	$E_{(TS-3)}$ /(a.u.)	$E_{CH3NO2...CH3NO2}$ /(a.u.)	$Ea_{(TS-3)}$ /(kJ/mol)
Z -0.010	-244.407667	-244.532254	327.10	-244.422794	287.39	-488.967368	-489.104419	359.83
Z -0.008	-244.409321	-244.532295	322.87	-244.423173	286.50	-488.968121	-489.097012	338.40
Z -0.006	-244.411193	-244.532326	318.03	-244.423445	285.87	-488.968979	-489.089803	317.22
Z -0.004	-244.413286	-244.532348	312.60	-244.423627	285.45	-488.969958	-489.080224	289.50
Z -0.002	-244.415603	-244.532362	306.55	-244.423740	285.19	-488.971021	-489.077643	279.94
Z +0.002	-244.420923	-244.532362	292.58	-244.423743	285.18	-488.971021	-489.077643	279.94
Z +0.004	-244.423939	-244.532348	284.63	-244.423645	285.40	-488.969958	-489.083129	297.13
Z +0.006	-244.427202	-244.532324	276.00	-244.423501	285.72	-488.968979	-489.089900	317.48
Z +0.008	-244.430723	-244.532291	266.67	-244.423296	286.16	-488.968104	-489.097014	338.45
Z +0.010	-244.434518	-244.532254	256.61	-244.423048	286.70	-488.967368	-489.104432	359.86
X -0.010	-244.422718	-244.534521	293.54	-244.423547	291.36			
X -0.008	-244.421554	-244.533746	294.56	-244.423629	289.11			
X -0.006	-244.420514	-244.533143	295.71	-244.423694	287.36	-488.971091	-489.080681	287.73
X -0.004	-244.419599	-244.532352	296.03	-244.423739	285.16	-488.971380	-489.078697	281.76
X -0.002	-244.418809	-244.532363	298.14	-244.423768	285.12	-488.971555	-489.077208	277.39
X +0.002	-244.417614	-244.532363	301.27	-244.423765	285.12	-488.971553	-489.077569	278.34
X +0.004	-244.417214	-244.532352	302.30	-244.423739	285.16	-488.971364	-489.081509	289.19
X +0.006	-244.416949	-244.533142	305.06	-244.423677	287.40	-488.971043	-489.086179	302.29
X +0.008	-244.416827	-244.533745	306.97	-244.423611	289.16	-488.970587	-489.091265	316.84
X +0.010	-244.416854	-244.534520	308.93	-244.423511	291.45	-488.969949	-489.096784	333.01
Y -0.010	-244.423983	-244.532264	284.29	-244.423659	285.14	-488.991158	-489.080778	235.30
Y -0.008	-244.422509	-244.532301	288.26	-244.423703	285.13	-488.986618	-489.079316	243.38
Y -0.006	-244.421189	-244.532330	291.80	-244.423734	285.12	-488.982384	-489.078141	251.41
Y -0.004	-244.420022	-244.532351	294.92	-244.423757	285.11	-488.978474	-489.077248	259.33
Y -0.002	-244.419008	-244.532366	297.62	-244.423771	285.11	-488.974885	-489.076640	267.16
Y +0.002	-244.417440	-244.532366	301.74	-244.423772	285.11	-488.968669	-489.076297	282.58
Y +0.004	-244.416886	-244.532351	303.15	-244.423756	285.12	-488.966041	-489.081863	304.09
Y +0.006	-244.416489	-244.532331	304.14	-244.423736	285.12	-488.963736	-489.087033	323.72
Y +0.008	-244.416249	-244.532301	304.69	-244.423703	285.12	-488.961709	-489.092592	343.63
Y +0.010	-244.416171	-244.532263	304.80	-244.423664	285.13	-488.960110	-489.098490	363.32

Table S3 The optimized geometrical parameters (Å) and AIM results (a.u.) of TS-2 in the different field strengths and orientations at the MP2/6-311++G(2d,p) level.

Field (a.u.)	$R_{C1\cdots H5}$	R_{N2-O4}	$R_{O4\cdots H5}$	$\rho_{C1\cdots H}$	ρ_{N2-O4}	$\rho_{O4\cdots H5}$	$\nabla^2\rho_{C1\cdots H5}$	$\nabla^2\rho_{N2-O4}$	$\nabla^2\rho_{O4\cdots H5}$
No Field	1.4752	1.3219	1.2461	0.1082	0.4072	0.1579	-0.0830	-0.5958	-0.2911
Z -0.0100	1.5003	1.3127	1.2123	0.1028	0.4162	0.1719	-0.0564	-0.6517	-0.4570
Z -0.0080	1.4948	1.3146	1.2189	0.1039	0.4143	0.1691	-0.0614	-0.6399	-0.4213
Z -0.0060	1.4898	1.3166	1.2255	0.1049	0.4124	0.1664	-0.0663	-0.6281	-0.3874
Z -0.0040	1.4850	1.3183	1.2321	0.1060	0.4107	0.1636	-0.0715	-0.6176	-0.3548
Z -0.0020	1.4800	1.3201	1.2392	0.1071	0.4090	0.1607	-0.0772	-0.6066	-0.3220
Z +0.0020	1.4703	1.3237	1.2536	0.1094	0.4055	0.1550	-0.0893	-0.5848	-0.2600
Z +0.0040	1.4657	1.3255	1.2608	0.1106	0.4037	0.1522	-0.0953	-0.5737	-0.2317
Z +0.0060	1.4614	1.3270	1.2675	0.1117	0.4022	0.1496	-0.1012	-0.5643	-0.2065
Z +0.0080	1.4570	1.3288	1.2748	0.1129	0.4005	0.1469	-0.1074	-0.5537	-0.1812
Z +0.0100	1.4523	1.3304	1.2822	0.1141	0.3989	0.1441	-0.1140	-0.5434	-0.1566
X -0.0100	1.4755	1.3067	1.2626	0.1094	0.4220	0.1508	-0.0963	-0.6650	-0.2242
X -0.0080	1.4749	1.3095	1.2595	0.1093	0.4192	0.1521	-0.0941	-0.6517	-0.2358
X -0.0060	1.4751	1.3125	1.2560	0.1090	0.4163	0.1536	-0.0913	-0.6380	-0.2496
X -0.0040	1.4750	1.3155	1.2526	0.1088	0.4134	0.1551	-0.0885	-0.6243	-0.2635
X -0.0020	1.4749	1.3186	1.2503	0.1086	0.4103	0.1561	-0.0866	-0.6097	-0.2734
X +0.0020	1.4751	1.3255	1.2429	0.1080	0.4038	0.1594	-0.0800	-0.5802	-0.3058
X +0.0040	1.4758	1.3291	1.2396	0.1076	0.4004	0.1609	-0.0768	-0.5652	-0.3211
X +0.0060	1.4756	1.3331	1.2380	0.1075	0.3967	0.1616	-0.0755	-0.5480	-0.3287
X +0.0080	1.4763	1.3370	1.2347	0.1071	0.3931	0.1632	-0.0720	-0.5322	-0.3453
X +0.0100	1.4770	1.3412	1.2318	0.1067	0.3892	0.1645	-0.0691	-0.5158	-0.3598
Y -0.0100	1.4772	1.3222	1.2498	0.1084	0.4069	0.1563	-0.0858	-0.5927	-0.2740
Y -0.0080	1.4770	1.3222	1.2486	0.1083	0.4070	0.1568	-0.0849	-0.5935	-0.2790
Y -0.0060	1.4767	1.3219	1.2467	0.1082	0.4072	0.1576	-0.0832	-0.5954	-0.2874
Y -0.0040	1.4762	1.3219	1.2465	0.1082	0.4073	0.1578	-0.0831	-0.5957	-0.2890
Y -0.0020	1.4760	1.3220	1.2478	0.1082	0.4071	0.1572	-0.0840	-0.5946	-0.2843
Y +0.0020	1.4749	1.3219	1.2455	0.1082	0.4072	0.1582	-0.0824	-0.5959	-0.2942
Y +0.0040	1.4739	1.3221	1.2458	0.1083	0.4070	0.1581	-0.0828	-0.5949	-0.2932
Y +0.0060	1.4743	1.3221	1.2446	0.1081	0.4070	0.1586	-0.0815	-0.5955	-0.2991
Y +0.0080	1.4732	1.3222	1.2447	0.1082	0.4070	0.1586	-0.0818	-0.5952	-0.2989
Y +0.0100	1.4724	1.3223	1.2444	0.1083	0.4068	0.1587	-0.0819	-0.5945	-0.2998

Table S4 part1 The optimized geometrical parameters (Å) and AIM results (a.u.) of TS-3 in the different field strengths and orientations at the MP2/6-311++G(2d,p) level.

Field	R_{N2-O4}	$R_{C1'\cdots H}$	$R_{O4\cdots H}$	ρ_{N2-O4}	$\rho_{C1'\cdots H}$	$\rho_{O4\cdots H}$	$\nabla^2\rho_{N2-O4}$	$\nabla^2\rho_{C1'\cdots H}$	$\nabla^2\rho_{O4\cdots H}$
No Field	1.3205	1.4565	1.1701	0.4048	0.1138	0.1875	-0.6129	-0.1282	-0.6114
Z-0.0100	1.3494	1.9043	1.0096	0.3932	0.1478	0.1440	-0.5595	-0.2845	-0.1269
Z-0.0080	1.3426	1.8308	1.0224	0.3957	0.1519	0.1412	-0.5618	-0.3064	-0.0978
Z-0.0060	1.3360	1.7583	1.0390	0.3983	0.1535	0.1408	-0.5672	-0.3150	-0.0888
Z-0.0040	1.3298	1.6788	1.0625	0.4009	0.1509	0.1444	-0.5754	-0.3013	-0.1132
Z-0.0020	1.3241	1.5790	1.1017	0.4035	0.1402	0.1564	-0.5900	-0.2466	-0.2221
Z+0.0020	1.3211	1.3741	1.2341	0.4022	0.0847	0.2284	-0.6253	-0.0284	-1.2387
Z+0.0040	1.3233	1.3423	1.2652	0.3973	0.0662	0.2579	-0.6205	0.0161	-1.6491
Z+0.0080	1.3426	1.8329	1.0221	0.3860	0.0453	0.2943	-0.5924	0.0478	-2.0818
X-0.0100	1.3074	1.4812	1.1537	0.4179	0.1059	0.1959	-0.6855	-0.0995	-0.7376
X-0.0080	1.3100	1.4752	1.1571	0.4153	0.1078	0.1940	-0.6704	-0.1058	-0.7087
X-0.0060	1.3125	1.4694	1.1607	0.4128	0.1095	0.1922	-0.6561	-0.1120	-0.6805
X-0.0040	1.3151	1.4634	1.1643	0.4102	0.1113	0.1903	-0.6415	-0.1188	-0.6516
X-0.0020	1.3178	1.4612	1.1664	0.4075	0.1122	0.1894	-0.6276	-0.1221	-0.6377
X+0.0020	1.3234	1.4543	1.1725	0.4021	0.1147	0.1864	-0.5985	-0.1318	-0.5960
X+0.0040	1.3261	1.4519	1.1751	0.3994	0.1156	0.1851	-0.5847	-0.1357	-0.5795
X+0.0060	1.3290	1.4523	1.1764	0.3967	0.1158	0.1847	-0.5714	-0.1365	-0.5750
X+0.0080	1.3318	1.4510	1.1786	0.3940	0.1164	0.1837	-0.5578	-0.1394	-0.5621
X+0.0100	1.3347	1.4557	1.1773	0.3913	0.1154	0.1846	-0.5457	-0.1354	-0.5769
Y-0.0100	1.3172	1.4441	1.1867	0.4062	0.1201	0.1773	-0.6098	-0.1570	-0.4737
Y-0.0080	1.3184	1.4436	1.1848	0.4063	0.1178	0.1808	-0.6134	-0.1468	-0.5190
Y-0.0060	1.3188	1.4443	1.1825	0.4060	0.1161	0.1831	-0.6141	-0.1395	-0.5514
Y-0.0040	1.3193	1.4488	1.1778	0.4056	0.1155	0.1844	-0.6136	-0.1364	-0.5685
Y-0.0020	1.3199	1.4532	1.1736	0.4052	0.1148	0.1859	-0.6130	-0.1328	-0.5881
Y+0.0020	1.3213	1.4593	1.1671	0.4045	0.1126	0.1894	-0.6132	-0.1228	-0.6382
Y+0.0040	1.3222	1.4609	1.1650	0.4042	0.1113	0.1914	-0.6134	-0.1174	-0.6666
Y+0.0060	1.3233	1.4635	1.1618	0.4040	0.1106	0.1924	-0.6132	-0.1141	-0.6826
Y+0.0080	1.3237	1.4652	1.1601	0.4035	0.1093	0.1942	-0.6125	-0.1090	-0.7096
Y+0.0100	1.3263	1.4673	1.1573	0.4035	0.1089	0.1948	-0.6133	-0.1069	-0.7178

Table S4 part2 The optimized geometrical parameters (Å) and AIM results (a.u.) of TS-3 in the different field strengths and orientations at the MP2/6-311++G(2d,p) level.

Field	$R_{N2'-O4'}$	$R_{C1\cdots H}$	$R_{H5\cdots O}$	$\rho_{N2'-O4'}$	$\rho_{C1\cdots H}$	$\rho_{H5\cdots O}$	$\nabla^2\rho_{N2'-O4'}$	$\nabla^2\rho_{C1\cdots H}$	$\nabla^2\rho_{H5\cdots O}$
Z-0.0100	1.3310	1.3433	1.2715	0.3800	0.0380	0.3072	-0.5751	0.0532	-2.2218
Z-0.0080	1.3284	1.3352	1.2769	0.3860	0.0455	0.2941	-0.5922	0.0477	-2.0788
Z-0.0060	1.3257	1.3334	1.2762	0.3918	0.0544	0.2784	-0.6082	0.0367	-1.8989
Z-0.0040	1.3233	1.3419	1.2656	0.3973	0.0660	0.2582	-0.6208	0.0165	-1.6531
Z-0.0020	1.3211	1.3725	1.2354	0.4022	0.0842	0.2290	-0.6258	-0.0271	-1.2485
Z+0.0020	1.3241	1.5763	1.1026	0.4035	0.1396	0.1569	-0.5904	-0.2439	-0.2280
Z+0.0040	1.3299	1.6773	1.0629	0.4009	0.1507	0.1446	-0.5757	-0.3003	-0.1147
Z+0.0080	1.3426	1.8329	1.0221	0.3957	0.1520	0.1411	-0.5617	-0.3070	-0.0968
X-0.0100	1.3378	1.4194	1.1913	0.3884	0.1246	0.1764	-0.5231	-0.1714	-0.4485
X-0.0080	1.3340	1.4269	1.1864	0.3920	0.1223	0.1789	-0.5420	-0.1615	-0.4833
X-0.0060	1.3306	1.4354	1.1810	0.3952	0.1197	0.1817	-0.5597	-0.1510	-0.5222
X-0.0040	1.3271	1.4437	1.1764	0.3985	0.1173	0.1841	-0.5780	-0.1415	-0.5587
X-0.0020	1.3237	1.4487	1.1741	0.4017	0.1159	0.1853	-0.5955	-0.1363	-0.5780
X+0.0020	1.3173	1.4616	1.1682	0.4079	0.1124	0.1885	-0.6300	-0.1236	-0.6290
X+0.0040	1.3144	1.4663	1.1664	0.4108	0.1112	0.1895	-0.6460	-0.1194	-0.6461
X+0.0060	1.3116	1.4684	1.1662	0.4136	0.1107	0.1896	-0.6610	-0.1180	-0.6493
X+0.0080	1.3088	1.4715	1.1661	0.4163	0.1100	0.1896	-0.6760	-0.1161	-0.6533
X+0.0100	1.3061	1.4679	1.1698	0.4189	0.1111	0.1876	-0.6892	-0.1209	-0.6261
Y-0.0100	1.3189	1.4382	1.1901	0.4079	0.1183	0.1791	-0.6196	-0.1500	-0.4985
Y-0.0080	1.3188	1.4449	1.1833	0.4067	0.1182	0.1800	-0.6151	-0.1487	-0.5090
Y-0.0060	1.3192	1.4503	1.1787	0.4064	0.1179	0.1811	-0.6147	-0.1466	-0.5228
Y-0.0040	1.3196	1.4519	1.1762	0.4060	0.1164	0.1835	-0.6147	-0.1397	-0.5552
Y-0.0020	1.3201	1.4537	1.1733	0.4054	0.1149	0.1857	-0.6141	-0.1333	-0.5858
Y+0.0020	1.3209	1.4602	1.1665	0.4042	0.1128	0.1891	-0.6113	-0.1238	-0.6337
Y+0.0040	1.3213	1.4638	1.1627	0.4033	0.1122	0.1902	-0.6079	-0.1208	-0.6493
Y+0.0060	1.3216	1.4659	1.1607	0.4023	0.1113	0.1918	-0.6046	-0.1165	-0.6726
Y+0.0080	1.3221	1.4699	1.1575	0.4020	0.1107	0.1927	-0.6040	-0.1138	-0.6865
Y+0.0100	1.3221	1.4701	1.1561	0.3995	0.1098	0.1942	-0.5927	-0.1099	-0.7068

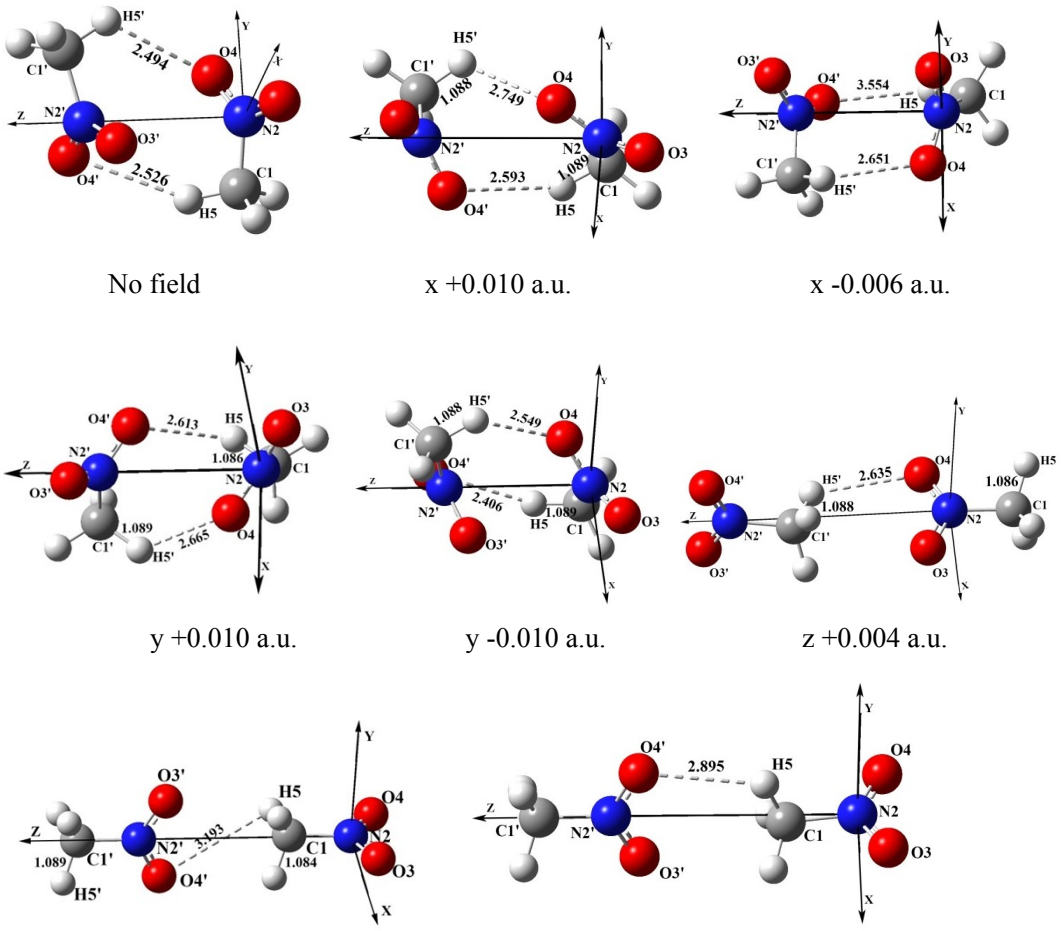

Fig. S1 Selected structures of the nitromethane dimer in the different external electric field strengths and orientations (including those in no field) at the MP2/6-311++G(2d,p) level (geometric parameters are in Å).