Electronic Supplementary Material (ESI) for New Journal of Chemistry.

SUPPLEMENTARY MATERIAL

Understanding the molecular mechanism of the stereoselective conversion of N-trialkylsilyloxy nitronates into bicyclic isoxazoline derivatives

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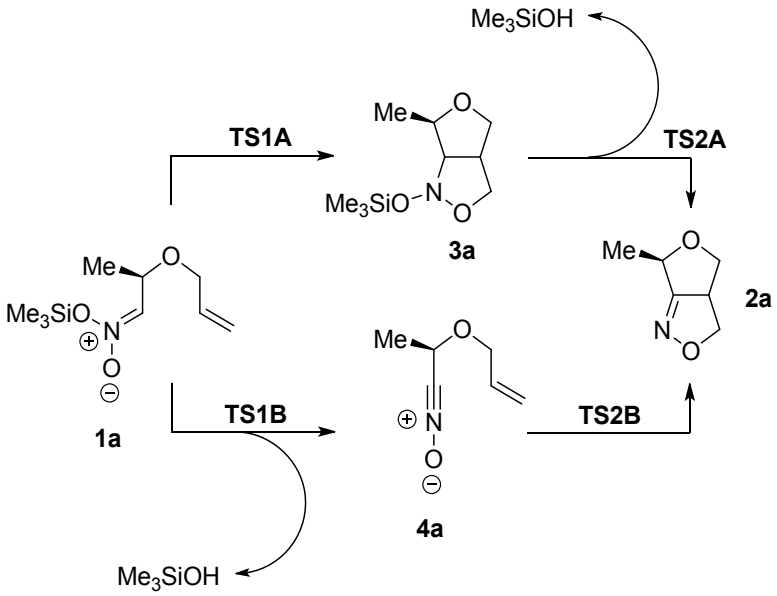
[1] Key structures for model reaction involving nitronate 1a



1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.455500	-0.981739	-0.162662
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3	6	0	3.262407	1.259684	-0.031307
4	6	0	2.021042	1.943708	0.466800
5	6	0	1.149372	-0.902576	0.566700
6	1	0	2.276223	-0.724683	-1.212684
7	1	0	4.147647	1.767498	0.360163
8	1	0	3.298489	1.308620	-1.129134
9	1	0	1.881104	1.950682	1.545595
10	1	0	1.069957	-1.105427	1.623983
11	6	0	1.138926	2.535051	-0.328523
12	1	0	0.265845	3.042184	0.066018
13	1	0	1.255138	2.522425	-1.407875
14	6	0	3.056379	-2.374979	-0.058742
15	1	0	2.375857	-3.116679	-0.482535
16	1	0	4.003717	-2.409491	-0.599392
17	1	0	3.244537	-2.627040	0.987865
18	8	0	-0.112443	-0.279619	-1.237890
19	7	0	0.053583	-0.576205	-0.038735
20	8	0	-1.060231	-0.522007	0.770034
21	14	0	-2.572994	-0.055139	0.054067
22	6	0	-2.507443	1.698896	-0.571122
23	1	0	-2.216090	2.384229	0.229517
24	1	0	-1.791074	1.793549	-1.388061
25	1	0	-3.495562	2.003669	-0.930786
26	6	0	-3.108646	-1.281313	-1.242739
27	1	0	-3.016739	-2.304046	-0.866561
28	1	0	-4.159638	-1.112151	-1.498225
29	1	0	-2.507950	-1.191282	-2.148421
30	6	0	-3.656069	-0.178681	1.568728
31	1	0	-4.689992	0.070499	1.310270
32	1	0	-3.647971	-1.189601	1.984103
33	1	0	-3.328193	0.513694	2.348272

TS1A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.529237	0.864126	-0.251487
2	8	0	-3.572607	0.101488	0.313887
3	6	0	-3.230720	-1.275335	0.223089
4	6	0	-1.771190	-1.514270	0.551899
5	6	0	-1.274253	0.498630	0.506259
6	1	0	-2.384989	0.598843	-1.307647
7	1	0	-3.892323	-1.800704	0.913116
8	1	0	-3.432885	-1.632648	-0.796416
9	1	0	-1.516913	-1.645764	1.600256
10	1	0	-1.190928	0.869911	1.522059
11	6	0	-0.943251	-2.085482	-0.394841
12	1	0	-0.004640	-2.544800	-0.112429
13	1	0	-1.315858	-2.319781	-1.384244
14	6	0	-2.885545	2.332079	-0.117733
15	1	0	-2.090408	2.954697	-0.532966
16	1	0	-3.813010	2.539032	-0.654646
17	1	0	-3.027909	2.592176	0.934079
18	8	0	-0.017813	-0.289627	-1.184000
19	7	0	-0.103299	0.396977	-0.128487
20	8	0	0.979975	0.317491	0.744898
21	14	0	2.553028	0.121255	0.073110
22	6	0	2.834934	-1.629060	-0.508493
23	1	0	2.589407	-2.345880	0.280388
24	1	0	2.222988	-1.854594	-1.383499
25	1	0	3.888144	-1.771437	-0.771450
26	6	0	2.808617	1.365475	-1.292562
27	1	0	2.668013	2.385587	-0.925060
28	1	0	3.824706	1.285420	-1.690995
29	1	0	2.105745	1.191768	-2.109910
30	6	0	3.611335	0.491996	1.563788
31	1	0	4.670238	0.370807	1.315437
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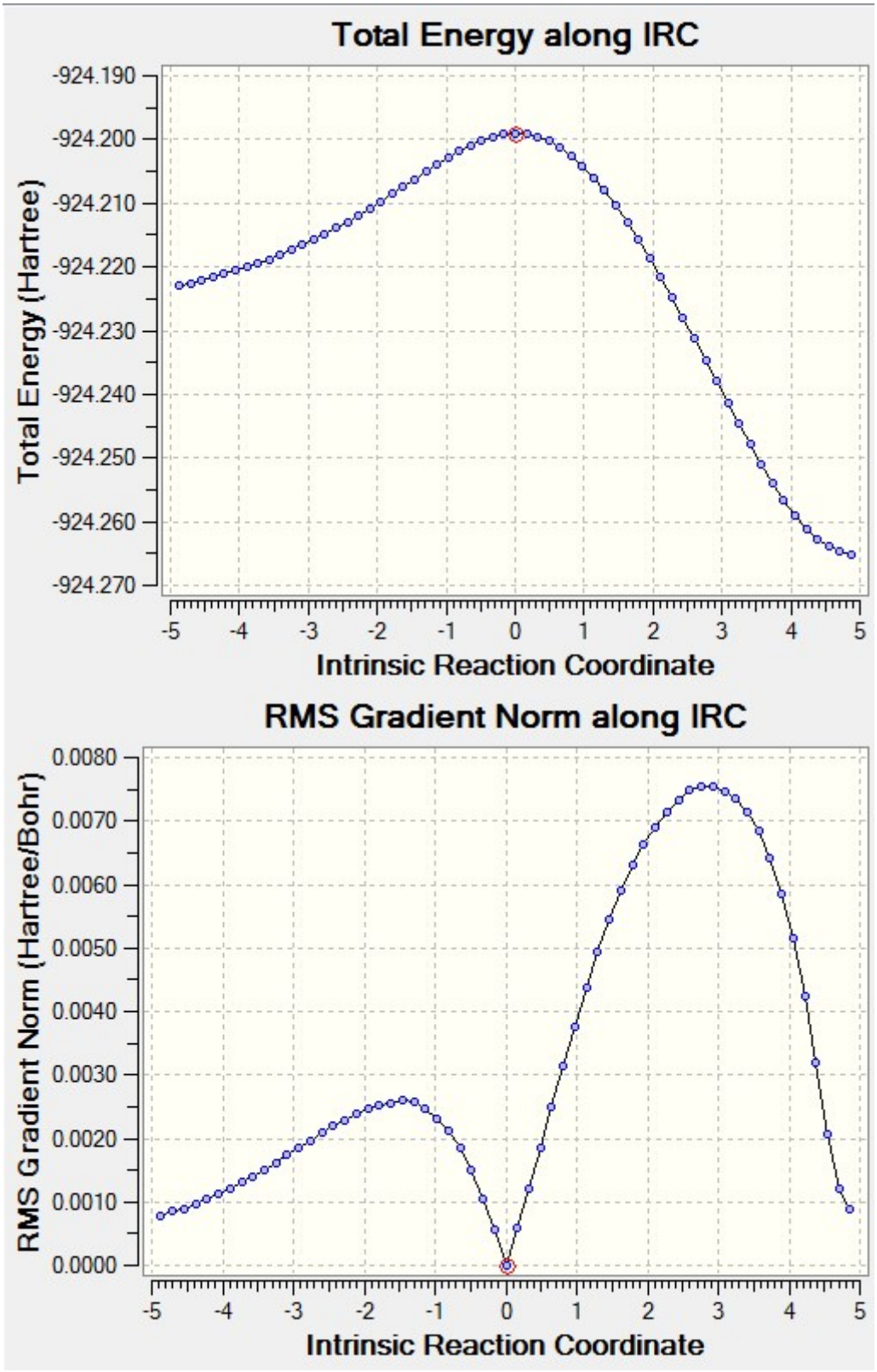
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-924.230
-924.240
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-924.270
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-3
-2
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1
2
3
4
5
Intrinsic Reaction Coordinate
RMS Gradient Norm along IRC
RMS Gradient Norm (Hartree/Bohr)
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0.0050
0.0040
0.0030
0.0020
0.0010
0.0000
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2
3
4
5
Intrinsic Reaction Coordinate

3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	-3.352181	-0.873641	0.103356
4	6	0	-1.974641	-1.124063	0.745631
5	6	0	-1.232509	0.206282	0.483314
6	1	0	-2.046413	0.832200	-1.401972
7	1	0	-4.183805	-1.272949	0.683555
8	1	0	-3.382156	-1.309115	-0.906478
9	1	0	-2.058851	-1.346548	1.808163
10	1	0	-0.908102	0.725052	1.382503
11	6	0	-1.089179	-2.125504	0.014738
12	1	0	-0.384977	-2.618182	0.688550
13	1	0	-1.637611	-2.871263	-0.560869
14	6	0	-2.176880	2.527005	-0.076266
15	1	0	-1.187613	2.913468	-0.333553
16	1	0	-2.922248	3.052369	-0.676015
17	1	0	-2.370501	2.731066	0.980113
18	8	0	-0.374777	-1.325982	-0.943636
19	7	0	-0.040062	-0.123817	-0.312732
20	8	0	0.995515	-0.414706	0.621761
21	14	0	2.493231	0.161027	0.043716
22	6	0	2.890854	-0.642048	-1.593465
23	1	0	2.976866	-1.726348	-1.485261
24	1	0	2.103409	-0.437438	-2.322859
25	1	0	3.836441	-0.261050	-1.991761
26	6	0	2.402573	2.020025	-0.124852
27	1	0	2.166164	2.492016	0.832986
28	1	0	3.355678	2.427179	-0.476169
29	1	0	1.629652	2.299391	-0.845463
30	6	0	3.692783	-0.354180	1.377037
31	1	0	4.709503	-0.045307	1.115199
32	1	0	3.439811	0.102893	2.337311
33	1	0	3.694586	-1.439826	1.505857

TS2A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.237894	1.268667	0.467669
2	8	0	3.519846	0.908225	-0.050299
3	6	0	3.565377	-0.482547	-0.302028
4	6	0	2.169464	-0.823284	-0.833610
5	6	0	1.315877	0.124423	0.006369
6	1	0	2.278357	1.290694	1.563234
7	1	0	4.369183	-0.667495	-1.013743
8	1	0	3.772461	-1.044444	0.622225
9	1	0	2.076062	-0.623077	-1.899177
10	1	0	0.271920	0.398670	-0.461085
11	6	0	1.578922	-2.159198	-0.459645
12	1	0	0.770311	-2.471441	-1.118754
13	1	0	2.274135	-2.974216	-0.268873
14	6	0	1.848967	2.627000	-0.073047
15	1	0	0.891126	2.936739	0.350605
16	1	0	2.606449	3.367230	0.190458
17	1	0	1.756874	2.588475	-1.160912
18	8	0	0.933115	-1.884750	0.846234
19	7	0	0.762938	-0.646083	1.045785
20	8	0	-1.103025	-0.227173	-0.273598
21	14	0	-2.691902	0.104826	-0.086433
22	6	0	-3.517141	-1.247162	0.936585
23	1	0	-3.435985	-2.218875	0.439694
24	1	0	-3.043533	-1.333331	1.919438
25	1	0	-4.580550	-1.036405	1.092495
26	6	0	-2.969452	1.746455	0.802806
27	1	0	-2.539456	2.580018	0.237551
28	1	0	-4.036213	1.952402	0.941347
29	1	0	-2.499517	1.736215	1.791544
30	6	0	-3.578641	0.202214	-1.749623
31	1	0	-4.644373	0.416461	-1.614992
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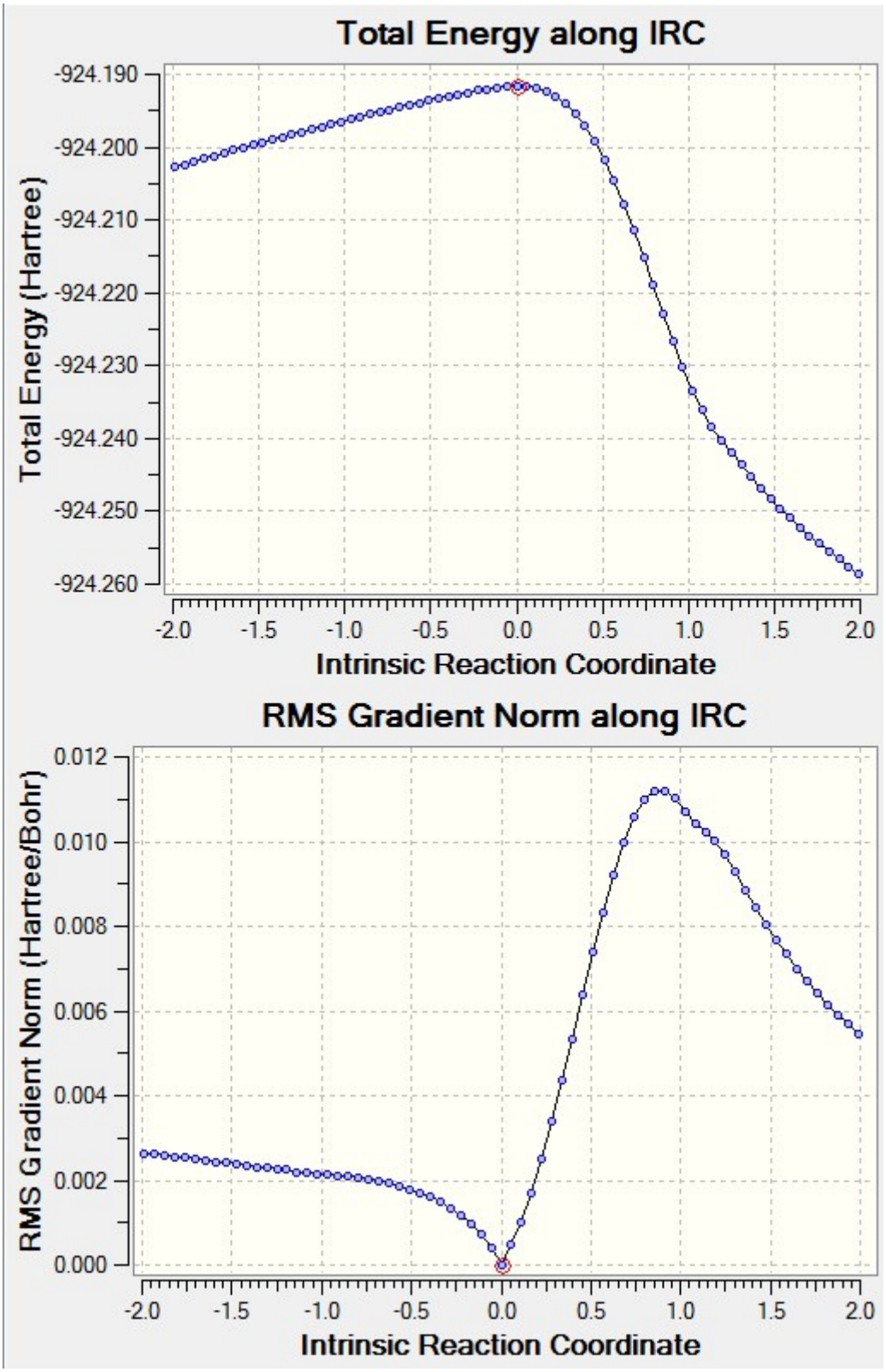
33	1	0	-3.492278	-0.743717	-2.293375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Total Energy (Hartree)
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-2.0
-1.5
-1.0
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0.0
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1.0
1.5
2.0
Intrinsic Reaction Coordinate
RMS Gradient Norm along IRC
RMS Gradient Norm (Hartree/Bohr)
0.012
0.010
0.008
0.006
0.004
0.002
0.000
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
Intrinsic Reaction Coordinate

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.376413	-0.342775	-0.416660
2	8	0	1.556473	1.069397	-0.226223
3	6	0	0.290408	1.728807	-0.161295
4	6	0	-0.620148	0.721593	0.539301
5	6	0	-0.070944	-0.531196	-0.073113
6	1	0	1.543153	-0.594915	-1.470354
7	1	0	0.440393	2.661738	0.380151
8	1	0	-0.088140	1.951845	-1.168593
9	1	0	-0.441234	0.733045	1.619590
10	6	0	-2.078921	0.513428	0.179174
11	1	0	-2.785804	0.784745	0.960041
12	1	0	-2.344242	1.016348	-0.758626
13	6	0	2.347184	-1.102378	0.468100
14	1	0	2.240677	-2.176625	0.302956
15	1	0	3.371554	-0.808641	0.231945
16	1	0	2.154738	-0.884228	1.520757
17	8	0	-2.189073	-0.920269	-0.022381
18	7	0	-0.927749	-1.400172	-0.406011

Me_3SiOH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.649960	-0.002063	2.216196
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3	14	0	-0.007230	-0.000085	0.034061
4	6	0	0.905692	1.533573	-0.536975
5	1	0	0.375818	2.443280	-0.240728
6	1	0	1.915837	1.579689	-0.117965
7	1	0	1.001757	1.540038	-1.627445
8	6	0	0.924795	-1.519903	-0.543147
9	1	0	0.406121	-2.437250	-0.250713
10	1	0	1.021823	-1.520974	-1.633529
11	1	0	1.935095	-1.554770	-0.123399
12	6	0	-1.759652	-0.009181	-0.604350
13	1	0	-1.776364	-0.005301	-1.698376
14	1	0	-2.294666	-0.898809	-0.261283
15	1	0	-2.306005	0.871079	-0.255018

TS1B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.645667	-0.956006	0.024456
2	8	0	-2.939268	-0.139418	-1.066952
3	6	0	-3.002416	1.257597	-0.788937
4	6	0	-1.663725	1.875652	-0.506274
5	6	0	-1.124169	-0.960751	0.259052
6	1	0	-3.134275	-0.579999	0.933295
7	1	0	-3.431829	1.692409	-1.693559
8	1	0	-3.695465	1.442196	0.043082
9	1	0	-0.890766	1.700512	-1.251221
10	1	0	-0.216941	-1.241627	-0.405390
11	6	0	-1.405292	2.616755	0.563625
12	1	0	-0.434179	3.074291	0.714840
13	1	0	-2.159826	2.800863	1.323650
14	6	0	-3.100224	-2.368310	-0.290957
15	1	0	-2.853930	-3.045680	0.528629
16	1	0	-4.180458	-2.367973	-0.443565
17	1	0	-2.614265	-2.721473	-1.201901
18	8	0	-0.357244	-0.083286	2.330033
19	7	0	-0.608938	-0.549516	1.300267
20	8	0	1.262189	-1.067121	0.047097
21	14	0	2.582667	-0.161379	-0.256143
22	6	0	2.143370	1.459123	-1.126112
23	1	0	1.633100	1.273152	-2.077248
24	1	0	1.480988	2.069121	-0.502464
25	1	0	3.037293	2.054448	-1.340660
26	6	0	3.430438	0.292236	1.367250
27	1	0	3.759360	-0.604553	1.900804
28	1	0	4.309506	0.921053	1.189775
29	1	0	2.753215	0.844957	2.026063
30	6	0	3.827481	-1.068340	-1.341771
31	1	0	4.707615	-0.446811	-1.538936
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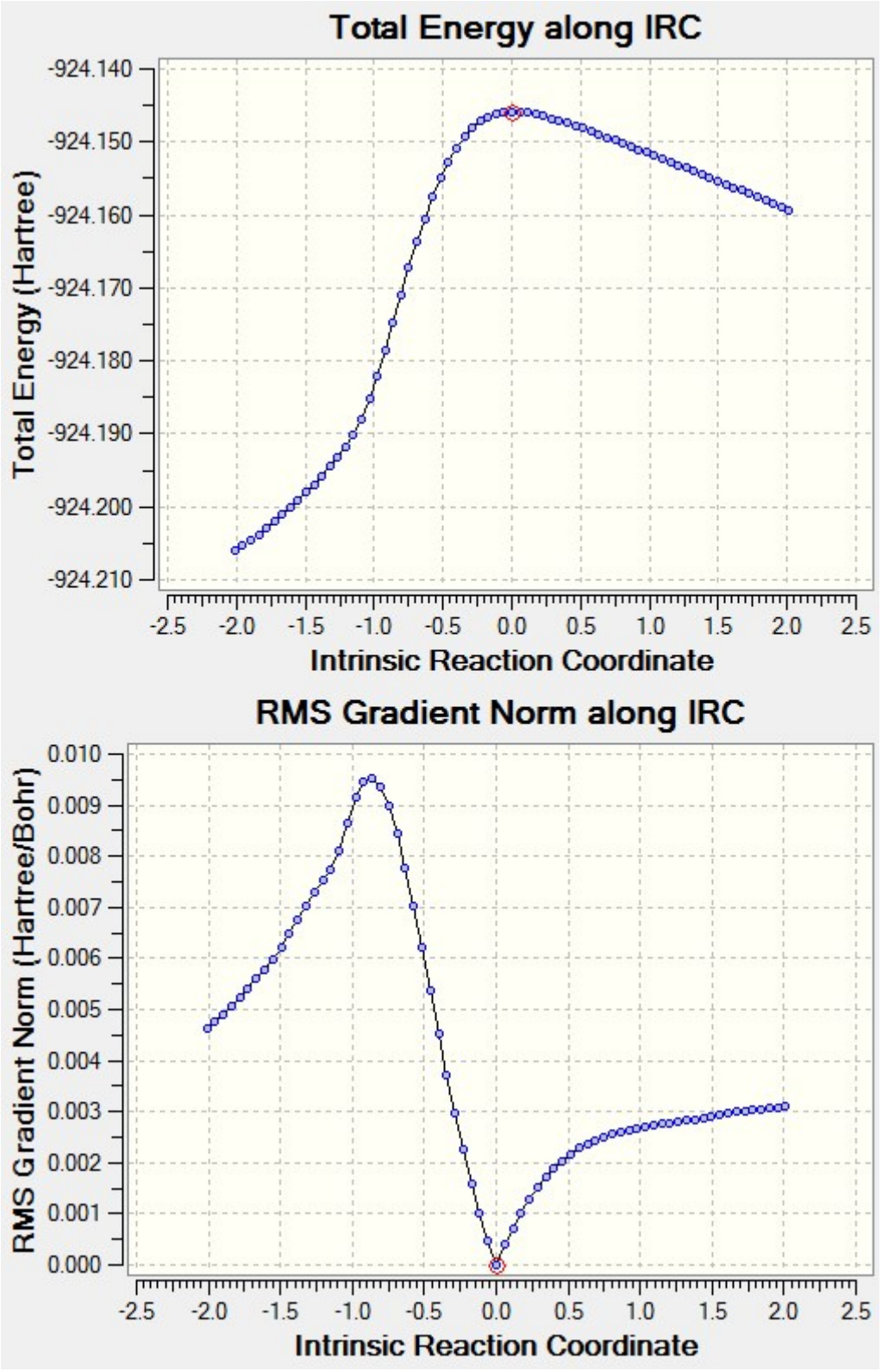
33	1	0	3.385811	-1.338421	-2.306073


Total Energy along IRC
Total Energy (Hartree)
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-2.5
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-1.5
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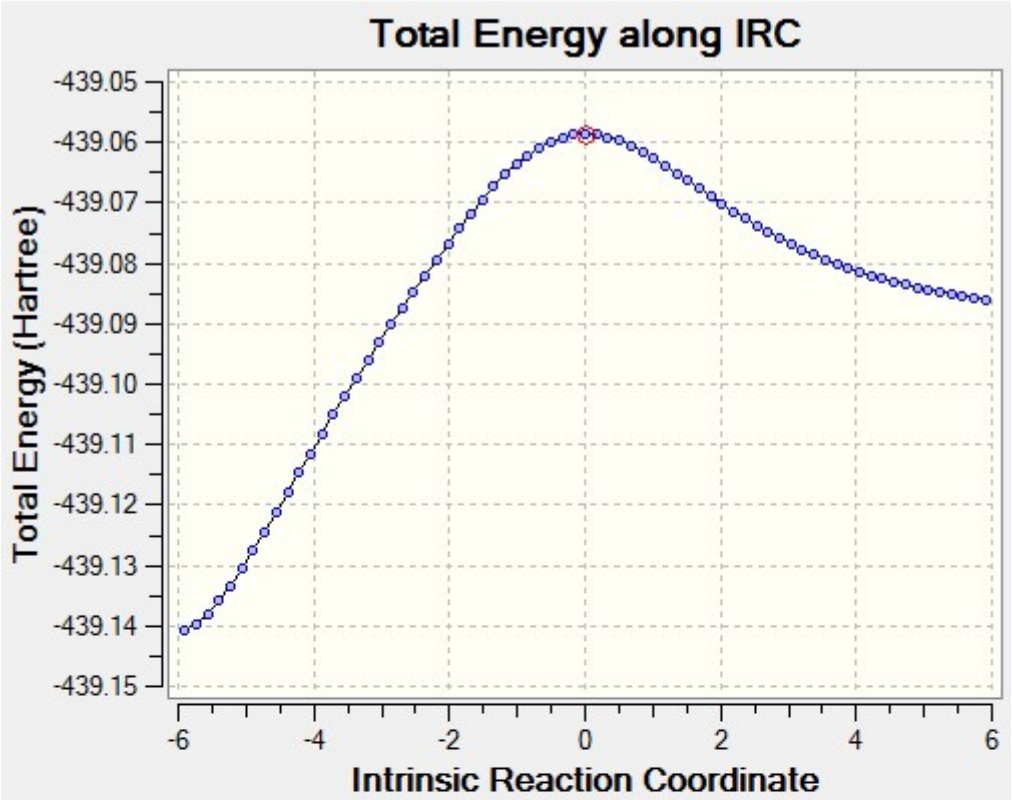
0.0
0.5
1.0
1.5
2.0
2.5
Intrinsic Reaction Coordinate
RMS Gradient Norm along IRC
RMS Gradient Norm (Hartree/Bohr)
0.010
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0.000
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
Intrinsic Reaction Coordinate

4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.514458	-1.097822	0.360879
2	8	0	-0.504743	-1.397453	-0.560873
3	6	0	-1.784845	-0.868516	-0.237824
4	6	0	-1.875391	0.623558	-0.373056
5	6	0	1.077940	0.255217	0.135899
6	1	0	0.109871	-1.109774	1.382719
7	1	0	-2.463149	-1.350242	-0.945538
8	1	0	-2.074706	-1.176265	0.776860
9	1	0	-1.557766	1.033200	-1.329094
10	6	0	-2.329595	1.424670	0.581410
11	1	0	-2.409162	2.495590	0.434305
12	1	0	-2.645173	1.033878	1.545153
13	6	0	1.595475	-2.160974	0.222507
14	1	0	2.412335	-1.971704	0.920951
15	1	0	1.158728	-3.137646	0.434204
16	1	0	1.988833	-2.161365	-0.795150
17	8	0	1.964110	2.413185	-0.225161
18	7	0	1.516715	1.308809	-0.039289

TS2B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.407096	-0.333638	-0.372919
2	8	0	1.492928	1.066487	-0.188972
3	6	0	0.235327	1.710933	-0.352184
4	6	0	-0.789996	1.076501	0.560318
5	6	0	0.011997	-0.724827	-0.010982
6	1	0	1.546029	-0.575698	-1.435895
7	1	0	0.413244	2.752979	-0.083154
8	1	0	-0.101619	1.671301	-1.397733
9	1	0	-0.497423	1.054858	1.608960
10	6	0	-2.115572	0.939967	0.268148
11	1	0	-2.847925	0.767475	1.044042
12	1	0	-2.492929	1.115221	-0.733365
13	6	0	2.477671	-1.006358	0.465859
14	1	0	2.466620	-2.085770	0.303709
15	1	0	3.455292	-0.614988	0.179257
16	1	0	2.309997	-0.800311	1.524162
17	8	0	-2.141346	-1.455054	-0.162717
18	7	0	-0.917583	-1.450284	-0.220844


Total Energy along IRC
Total Energy (Hartree)
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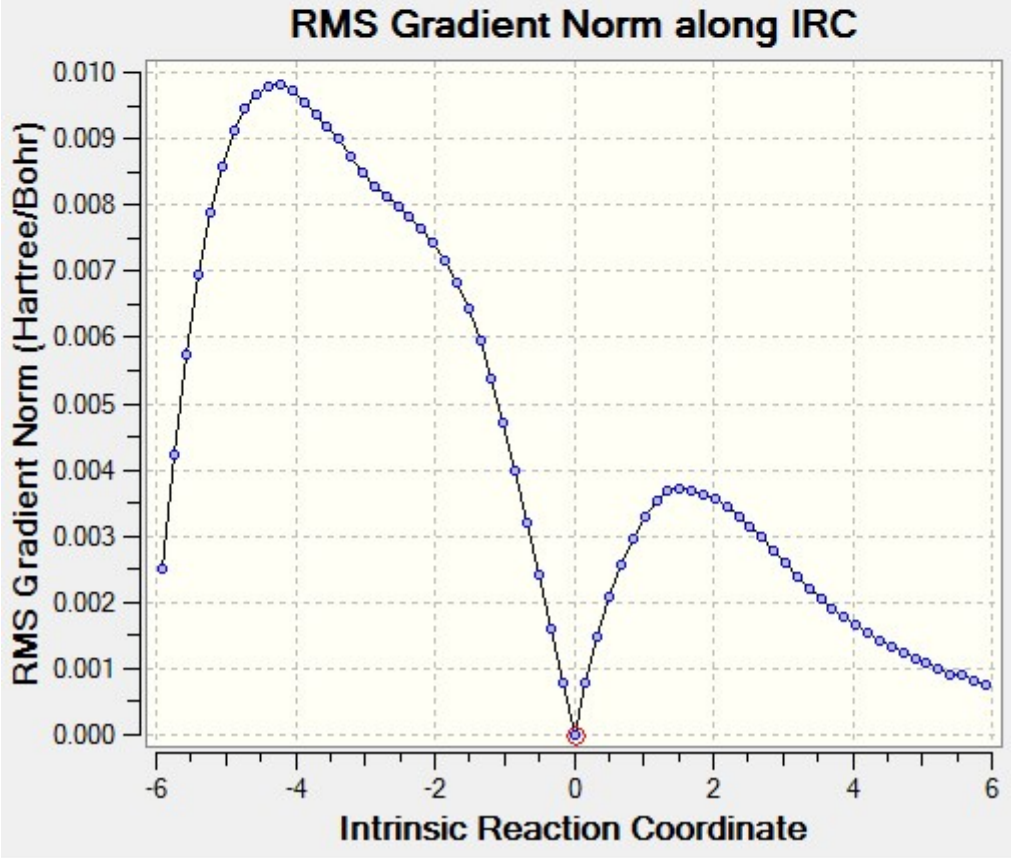
-439.08
-439.09
-439.10
-439.11
-439.12
-439.13
-439.14
-439.15
-6
-4
-2
0
2
4
6
Intrinsic Reaction Coordinate


RMS Gradient Norm along IRC
RMS Gradient Norm (Hartree/Bohr)
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0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0.000
-6
-4
-2
0
2
4
6
Intrinsic Reaction Coordinate

[2] Energetical parameters and geometrical parameters for key structures of domino-reactions leading from nitronates 1a-e into respective isoxazoline systems 2a-e according the ωB97XD(PCM)/6-311G(d,p) calculations

Table S1. Energetical parameters of domino-reactions leading from nitronates **1a-e** into respective isoxazoline systems **2a-e** according the ωB97XD(PCM)/6-311G(d,p) calculations (ΔH, ΔG are in kcal/mol; ΔS are in cal/molK).

Solvent	R	X	Path	Transition	ΔH	ΔS	ΔG
Benzene	Me	O	**A**	**1a→TS1A**	16.5	-8.7	19.1
				1a→3a	-25.9	-9.5	-23.0
				1a→TS2A	19.1	-9.7	22.0
				1a→2a+Me_3SiOH	-38.8	35.0	-49.3
			B	**1a→TS1B**	46.8	5.4	45.2
				1a→4a+Me_3SiOH	-7.4	50.5	-22.5
				1a→TS2B	11.2	39.3	-0.5
Acetone	Me	O	**A**	**1a→TS1A**	16.7	-10.0	19.7
				1a→3a	-26.1	-9.0	-23.5
				1a→TS2A	16.9	-6.4	18.8
				1a→2a+Me_3SiOH	-41.5	34.3	-51.7
			B	**1a→TS1B**	44.6	4.5	43.2
				1a→4a+Me_3SiOH	-9.7	49.0	-24.3
				1a→TS2B	9.4	38.8	-2.2
Nitromethane	Me	O	**A**	**1a→TS1A**	16.8	-10.3	19.8
				1a→3a	-26.2	-9.1	-23.5
				1a→TS2A	16.6	-6.4	18.5
				1a→2a+Me_3SiOH	-41.6	34.1	-51.8
			B	**1a→TS1B**	44.4	4.1	43.2
				1a→4a+Me_3SiOH	-9.8	48.7	-24.4
				1a→TS2B	9.2	38.5	-2.2
Water	Me	O	**A**	**1a→TS1A**	16.8	-10.7	20.0
				1a→3a	-26.2	-8.9	-23.5
				1a→TS2A	16.5	-6.4	18.4
				1a→2a+Me_3SiOH	-41.7	33.7	-51.8
			B	**1a→TS1B**	44.3	4.0	43.1
				1a→4a+Me_3SiOH	-9.9	48.4	-24.4
				1a→TS2B	9.2	38.2	-2.2
Benzene	Me	S	**A**	**1b→TS1A**	20.0	-11.7	23.5
				1b→3b	-23.7	-11.7	-20.2
				1b→TS2A	19.7	-8.4	22.1
				1b→2b+Me_3SiOH	-41.7	34.7	-52.1
			B	**1b→TS1B**	48.2	5.1	46.7
				1b→4b+Me_3SiOH	-7.2	44.7	-20.5
				1b→TS2B	12.1	38.5	0.6
Benzene	i-Pr	S	**A**	**1c→TS1A**	19.7	-11.9	23.2
				1c→3c	-24.4	-13.6	-20.4
				1c→TS2A	17.5	-9.8	20.5

				1c→2c+Me_3SiOH	-45.8	32.3	-55.4
			B	**1c→TS1B**	46.9	0.8	46.7
				1c→4c+Me_3SiOH	-9.8	46.5	-23.7
				1c→TS2B	8.2	35.7	-2.5
Benzene	Ph	S	**A**	**1d→TS1A**	19.7	-6.5	21.6
				1d→3d	-25.8	-8.5	-23.3
				1d→TS2A	18.0	-7.9	20.4
				1d→2d+Me_3SiOH	-43.9	39.0	-55.5
			B	**1d→TS1B**	48.2	5.4	46.6
				1d→4d+Me_3SiOH	-8.6	50.6	-23.7
				1d→TS2B	10.1	41.0	-2.1
Benzene	NO_2	S	**A**	**1e→TS1A**	20.6	-10.4	23.7
				1e→3e	-24.4	-12.2	-20.7
				1e→TS2A	17.3	-10.8	20.5
				1e→2e+Me_3SiOH	-45.4	34.3	-55.7
			B	**1e→TS1B**	52.7	10.4	49.6
				1e→4e+Me_3SiOH	-7.6	46.0	-21.3
				1e→TS2B	10.3	38.2	-1.1

Table S2. Geometrical parameters for key structures of domino-reactions leading from nitronates **1a-e** into respective isoxazoline systems **2a-e** according the ωB97XD(PCM)/6-311G(d,p) calculations.

Solvent	R	X	Structure	Interatomic distance [Å]							
				O1-N2	N2-C3	C3-C4	C4-C5	C5-O1	N2-O6	O6-H7	H7-C3
Benzene	Me	O	**1a**	1.246	1.294	2.978	1.327	3.212	1.378	2.368	1.079
			TS1A	1.262	1.336	2.074	1.381	2.169	1.394	2.371	1.085
			3a	1.398	1.471	1.546	1.524	1.438	1.425	2.346	1.088
			TS2A	1.266	1.407	1.527	1.508	1.482	2.323	1.522	1.176
			Me_3SiOH							0.956	
			2a	1.403	1.265	1.499	1.517	1.452			
			TS1B	1.158	1.232	2.987	1.327	3.392	2.311	1.557	1.159
			4a	1.206	1.155	3.019	1.326	4.479			
			TS2B	1.225	1.198	2.053	1.364	2.434			
Acetone	Me	O	**1a**	1.249	1.293	2.976	1.327	3.290	1.377	2.371	1.080
			TS1A	1.263	1.336	2.072	1.381	2.176	1.394	2.373	1.085
			3a	1.398	1.472	1.545	1.523	1.441	1.425	2.349	1.088
			TS2A	1.254	1.411	1.528	1.507	1.494	2.440	1.607	1.159
			Me_3SiOH							0.957	
			2a	1.406	1.265	1.497	1.516	1.516			
			TS1B	1.153	1.232	3.035	1.327	3.384	2.390	1.648	1.138
			4a	1.211	1.153	3.032	1.327	4.529			
			TS2B	1.230	1.197	2.044	1.364	2.466			
Nitro-methane	Me	O	**1a**	1.249	1.293	2.975	1.327	3.295	1.376	2.371	1.080
			TS1A	1.263	1.336	2.072	1.381	2.176	1.394	2.373	1.085
			3a	1.398	1.472	1.545	1.523	1.441	1.425	2.349	1.088
			TS2A	1.253	1.412	1.528	1.506	1.495	2.448	1.614	1.157

			Me_3SiOH							0.957	
			2a	0.957	1.265	1.497	1.516	1.455			
			TS1B	1.153	1.232	3.039	1.327	3.377	2.398	1.659	1.135
			4a	1.212	1.153	3.032	1.327	4.530			
			TS2B	1.231	1.197	2.044	1.364	2.469			
Water	Me	O	**1a**	1.249	1.293	2.975	1.327	3.301	1.376	2.371	1.080
			TS1A	1.264	1.336	2.072	1.381	2.177	1.394	2.373	1.085
			3a	1.398	1.472	1.545	1.523	1.441	1.425	2.350	1.088
			TS2A	1.252	1.412	1.528	1.506	1.495	2.455	1.620	1.156
			Me_3SiOH							0.957	
			2a	1.406	1.265	1.497	1.516	1.455			
			TS1B	1.152	1.232	3.041	1.327	3.371	2.403	1.667	1.134
			4a	1.212	1.153	3.033	1.327	4.531			
			TS2B	1.231	1.197	2.043	1.364	2.470			
Benzene	Me	S	**1b**	1.251	1.294	3.341	1.327	3.328	1.374	2.366	1.079
			TS1A	1.264	1.340	2.109	1.383	2.143	1.394	2.370	1.085
			3b	1.398	1.476	1.551	1.527	1.437	1.425	2.333	1.088
			TS2A	1.270	1.412	1.528	1.512	1.478	2.275	1.518	1.185
			2b	1.393	1.267	1.501	1.524	1.450			
			TS1B	1.159	1.236	3.154	1.327	3.211	2.299	1.533	1.166
			4b	1.207	1.154	3.166	1.327	4.170			
			TS2B	1.225	1.198	2.120	1.364	2.365			
Benzene	i-Pr	S	**1c**	1.252	1.294	3.338	1.327	3.331	1.374	2.362	1.079
			TS1A	1.264	1.340	2.103	1.383	2.149	1.395	2.364	1.083
			3c	1.398	1.477	1.551	1.526	1.436	1.425	2.314	1.087
			TS2A	1.270	1.413	1.526	1.511	1.479	2.276	1.524	1.183
			2c	1.391	1.268	1.501	1.525	1.450			
			TS1B	1.160	1.236	3.208	1.327	3.210	2.306	1.535	1.165
			4c	1.208	1.154	3.210	1.327	4.443			
			TS2B	1.224	1.198	2.121	1.364	2.363			
Benzene	Ph	S	**1d**	1.251	1.294	3.349	1.327	3.330	1.373	2.368	1.078
			TS1A	1.263	1.339	2.106	1.383	2.147	1.392	2.375	1.084
			3d	1.394	1.473	1.549	1.529	1.438	1.425	2.344	1.087
			TS2A	1.270	1.413	1.529	1.513	1.478	2.263	1.526	1.175
			2d	1.389	1.266	1.499	1.526	1.451			
			TS1B	1.159	1.235	3.100	1.327	3.235	2.298	1.525	1.166
			4d	1.206	1.154	3.149	1.327	3.947			
			TS2B	1.223	1.200	2.123	1.365	2.349			
Benzene	NO_2	S	**1e**	1.241	1.301	3.299	1.327	3.133	1.364	2.387	1.077
			TS1A	1.260	1.341	2.117	1.384	2.123	1.383	2.390	1.082
			3e	1.397	1.474	1.548	1.527	1.436	1.418	2.333	1.086
			TS2A	1.271	1.416	1.525	1.518	1.476	2.207	1.448	1.212
			2e	1.371	1.267	1.497	1.528	1.458			
			TS1B	1.158	1.238	4.395	1.329	5.236	2.208	1.451	1.194
			4e	1.194	1.155	4.358	1.329	6.889			
			TS2B	1.213	1.197	2.126	1.362	2.442			

[3] Energetical parameters for key structures of domino-reactions leading from nitronate 1a into isoxazoline 2a according the different calculations

Table S3. Kinetic and thermodynamic parameters of domino-reactions leading from nitronate **1a** into isoxazoline **2a** computed at 25ºC in benzene, according to different functionals and basic sets (ΔH and ΔG values are in kcal/mol; ΔS values are in cal·mol^{-1}·K^{-1}).

Functional	Basic set	Path		ΔH	ΔG	ΔS
ωB97XD	6-31G(d)	A	**1a→TS1A**	15.1	18.1	-10.2
			1a→3a	-30.1	-26.9	-10.7
			1a→TS2A	18.2	20.0	-6.0
			1a→2a+Me_3SiOH	-37.4	-47.7	34.6
		B	**1a→TS1B**	50.9	49.4	4.9
			1a→4a+Me_3SiOH	-1.2	-15.9	49.1
			4a→TS2B	17.4	20.4	-10.2
	6-31++G(d,p)	A	**1a→TS1A**	16.2	18.7	-8.5
			1a→3a	-28.0	-25.3	-9.1
			1a→TS2A	18.3	20.2	-6.3
			1a→2a+Me_3SiOH	-41.4	-52.0	35.4
		B	**1a→TS1B**	49.3	47.5	6.2
			1a→4a+Me_3SiOH	-6.6	-21.5	50.0
			4a→TS2B	17.8	20.7	-9.9
MPWB1K	6-31G(d)	A	**1a→TS1A**	14.8	18.2	-11.4
			1a→3a	-34.1	-30.7	-11.6
			1a→TS2A	18.2	20.0	-5.9
			1a→2a+Me_3SiOH	-43.6	-54.0	34.8
		B	**1a→TS1B**	55.0	54.0	3.5
			1a→4a+Me_3SiOH	-4.2	-18.0	48.3
			4a→TS2B	17.9	20.8	-9.8
	6-311G(d,p)	A	**1a→TS1A**	15.7	18.3	-8.6
			1a→3a	-30.8	-27.8	-10.2
			1a→TS2A	18.2	18.6	-1.1
			1a→2a+Me_3SiOH	-45.9	-56.9	36.7
		B	**1a→TS1B**	50.5	48.0	8.5
			1a→4a+Me_3SiOH	-9.7	-24.8	50.8
			4a→TS2B	18.9	21.9	-10.2
	6-31++G(d,p)	A	**1a→TS1A**	15.7	18.8	-10.5
			1a→3a	-32.1	-28.8	-11.2
			1a→TS2A	18.1	19.0	-3.0
			1a→2a+Me_3SiOH	-48.0	-58.7	35.9
		B	**1a→TS1B**	53.2	51.4	6.1
			1a→4a+Me_3SiOH	-9.5	-24.4	50.1
			4a→TS2B	18.3	21.3	-10.0
B3LYP	6-31G(d)	A	**1a→TS1A**	15.4	18.7	-10.9
			1a→3a	-22.2	-18.3	-13.0
			1a→TS2A	17.9	19.9	-6.5
			1a→2a+Me_3SiOH	-36.7	-46.1	31.2
		B	**1a→TS1B**	42.4	40.7	5.8

		1a→4a+Me_3SiOH	-8.0	-21.9	46.4
		4a→TS2B	16.4	19.8	-11.4
6-311G(d,p)	A	**1a→TS1A**	17.1	20.6	-11.9
		1a→3a	-17.3	-13.3	-13.4
		1a→TS2A	19.9	22.2	-7.8
		1a→2a+Me_3SiOH	-38.1	-47.2	30.6
	B	**1a→TS1B**	40.5	39.7	4.3
		1a→4a+Me_3SiOH	-14.5	-28.2	46.0
		4a→TS2B	17.7	21.2	-11.6
6-31++G(d,p)	A	**1a→TS1A**	16.7	20.5	-12.5
		1a→3a	-19.5	-15.3	-14.0
		1a→TS2A	19.7	19.2	-6.3
		1a→2a+Me_3SiOH	-41.1	-50.2	30.3
	B	**1a→TS1B**	41.8	40.5	5.2
		1a→4a+Me_3SiOH	-14.2	-27.7	45.5
		4a→TS2B	16.9	20.1	-10.7