

Efficient production of lactic acid from sugars over Sn-Beta zeolite in water:

Catalytic performance and mechanistic insights

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Supporting Information:

Complete lists for refs. 16, 30 and 37, and Cartesian coordinates for the optimized structures in Figure 7

Complete lists for refs. 16, 30 and 37:

Ref. 16: Clippel, F.; Dusselier, M.; Rompaey, R.; Vanelderen, P.; Dijkmans, J.; Makshina, E.; Giebel, L.; Oswald, S.; Baron, G.; Denayer, J.; Pescarmona, P.; Jacobs, P.; Sels, B. Fast and selective sugar conversion to alkyl lactate and lactic acid with bifunctional carbon–silica catalysts. *J. Am. Chem. Soc.* 2012, *134*, 10089-10101.

Ref. 30: Bermejo-Deval, R.; Assary, R. S.; Nikolla, E.; Moliner, M.; Roman-Leshkov, Y.; Hwang, S. J.; Palsdottir, A.; Silverman, D.; Lobo, R. F.; Curtiss, L. A.; Davis, M. E. Metalloenzyme-like catalyzed isomerizations of sugars by Lewis acid zeolites. *Proc. Natl. Acad. Sci.* **2012**, *109*, 9727-9732.

Ref. 37: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, 2009.

Cartesian coordinates for the optimized structures in Figure 7:

GLY

C	-0.105919	0.455353	0.460155
O	0.506004	1.589847	-0.169241
C	-1.220852	-0.118603	-0.414566
H	-1.043844	-0.053485	-1.507784
O	-2.237249	-0.612162	0.041800
C	1.013887	-0.576691	0.666361
H	1.741205	-0.152885	1.372772
H	0.595111	-1.488558	1.099166
O	1.638500	-0.946681	-0.559238
H	-0.535042	0.709018	1.438059
H	1.992627	-0.138446	-0.959556
H	-0.130779	2.315973	-0.220928

IM-1

C	-0.119372	0.542179	0.541473
O	0.706789	1.427874	-0.237970
C	-1.461436	0.315087	-0.197376
H	-1.882196	1.212453	-0.687990
O	-1.996867	-0.770489	-0.213269
C	0.669054	-0.769427	0.702014
H	1.379308	-0.755665	1.528651
H	0.019424	-1.643890	0.700997
O	1.470570	-0.826708	-0.580900
H	2.298436	-1.341856	-0.524665
H	-0.341009	0.953983	1.531695
H	1.619101	0.155535	-0.797413
H	0.933519	2.246986	0.229160

TS-1

C	-0.006158	-0.236218	0.439512
O	0.164418	-1.089234	1.493872
C	-0.265021	1.261776	0.717640
H	-0.134483	1.567380	1.773465
O	-0.582070	2.020263	-0.167133
C	0.566925	-0.587196	-0.786108
H	0.818272	-1.623299	-0.989351
H	0.503370	0.129354	-1.598301
O	2.773511	-0.124004	-0.588979
H	3.301121	0.265311	-1.304813
H	-0.974631	-0.549251	-0.282794
H	3.362099	-0.734243	-0.116447
H	-0.426530	-0.867524	2.231980

O	-2.598039	-0.720119	-0.747096
H	-3.159606	-1.510737	-0.735173
H	-3.126651	-0.002409	-1.130145

IM-2

C	0.464125	-0.067275	0.000067
O	1.431739	-0.905331	-0.000115
C	-0.988847	-0.602883	0.000197
H	-1.105236	-1.705354	0.000621
O	-1.904568	0.179555	-0.000192
C	0.757264	1.362967	0.000042
H	1.826966	1.567847	-0.001113
H	0.252015	1.819234	-0.866056
H	1.159537	-1.851525	-0.000191
H	0.254095	1.819143	0.867358

PAL

C	0.525242	-0.177352	-0.000023
O	1.334154	-1.094627	0.000025
C	-0.970161	-0.555317	-0.000026
H	-1.146619	-1.649851	-0.000048
O	-1.868839	0.265125	0.000020
C	0.877112	1.287797	-0.000011
H	0.436081	1.773245	0.877079
H	1.960486	1.408180	-0.001026
H	0.434378	1.773682	-0.876008

TS-2

C	0.877985	-0.181617	0.074568
O	1.624031	-1.143950	0.178478
C	-0.601000	-0.368183	0.478144
H	-0.780010	-1.394550	0.837666
O	-1.295687	0.639264	0.959930
C	1.301894	1.191010	-0.380413
H	1.044053	1.925843	0.388005
H	2.372740	1.197115	-0.584079
H	0.743387	1.465957	-1.281734
O	-1.449947	-0.300555	-1.018529
H	-2.028033	-1.074243	-1.144231
H	-1.852586	0.474548	-0.208457

TS-2-LA

C	2.735502	0.571811	-0.237512
O	3.899270	0.685159	-0.586935
C	2.354161	-0.806899	0.361903
H	3.208864	-1.487931	0.315678
O	1.606225	-0.903721	1.424014
C	1.713316	1.674731	-0.301915

H	1.104585	1.724212	0.604543
H	2.223715	2.621755	-0.478874
H	1.030607	1.480490	-1.137194
O	1.380250	-1.430197	-1.005738
H	1.454121	-2.399506	-1.006567
H	0.583427	-0.608071	1.172652
C	-1.486901	0.233642	0.396780
C	-2.657806	0.020964	-0.569730
H	-2.237272	-0.093057	-1.579174
C	-3.443512	-1.251147	-0.208301
H	-4.280702	-1.362748	-0.902129
H	-2.805124	-2.137211	-0.270173
H	-3.845675	-1.171549	0.805822
O	-0.524484	-0.674927	0.343121
H	0.419861	-1.181566	-0.656655
O	-3.500943	1.162428	-0.556837
H	-3.179525	1.713311	0.180902
O	-1.480998	1.191666	1.170353

IM-3

C	0.717675	-0.281317	-0.026023
O	0.825934	-1.421590	0.403407
C	-0.697780	0.233993	-0.389848
H	-0.723813	0.593678	-1.428698
O	-1.639824	-0.786333	-0.267173
C	1.872436	0.667804	-0.201385
H	1.682867	1.574639	0.381114
H	2.802075	0.194335	0.115105
H	1.944283	0.971774	-1.252107
O	-0.931176	1.321189	0.506792
H	-1.879140	1.518677	0.468526
H	-1.219725	-1.482112	0.275391

IM-4

O	-2.322664	0.287577	-1.015117
O	-0.643187	-1.889967	0.260146
Si	-3.721675	-0.578540	-1.203794
H	-4.234467	-1.085329	0.097749
H	-4.736715	0.327012	-1.802157
H	-3.519440	-1.738512	-2.114268
Si	0.164153	-3.047687	1.129608
H	0.371147	-2.628354	2.541593
H	-0.663262	-4.278517	1.098364
H	1.494160	-3.342242	0.529936
O	-0.585658	1.337774	1.320360
Si	-1.729012	2.390079	1.913468

H	-2.986846	1.680279	2.266252
H	-1.154946	3.006437	3.135838
H	-2.042440	3.456728	0.926597
O	0.480207	0.638517	-1.803478
SN	-0.535076	0.034154	-0.159358
C	2.859113	0.011878	0.412619
O	1.654612	-0.207025	0.604416
C	3.381591	0.752878	-0.849483
H	4.457501	0.911184	-0.741705
O	3.204965	-0.104998	-1.952805
C	3.878468	-0.469230	1.399186
H	4.426271	0.396745	1.790437
H	3.408960	-1.018831	2.214388
H	4.611868	-1.098195	0.881223
O	2.794486	2.016468	-0.973808
H	2.244704	-0.126420	-2.144508
H	-0.152798	0.855664	-2.506902
H	1.864489	1.880798	-1.246540

TS-3

O	2.361569	0.262233	-0.269732
O	0.512507	-1.994216	-0.174275
SI	3.582685	-0.696606	-0.862244
H	3.216579	-1.307406	-2.167725
H	4.764643	0.183048	-1.060690
H	3.945392	-1.780060	0.089070
SI	-0.537590	-3.266278	-0.133976
H	0.113057	-4.418759	-0.807188
H	-0.900735	-3.653589	1.255525
H	-1.806083	-2.957607	-0.861826
O	0.094165	1.925276	0.453253
SI	0.989653	3.263026	0.052763
H	1.404062	3.256633	-1.375505
H	0.116166	4.448223	0.281087
H	2.199769	3.402378	0.905342
O	0.181051	-0.198638	2.391527
SN	0.478854	-0.055016	0.282076
C	-2.195156	0.538451	-1.103606
O	-1.038643	0.259259	-1.448040
C	-2.588738	0.477873	0.404665
H	-2.543742	1.508781	0.782273
O	-3.920298	0.033964	0.561466
C	-3.225602	0.954513	-2.102047
H	-3.684992	1.895483	-1.779963
H	-2.780355	1.058053	-3.091140

H	-4.032234	0.214426	-2.114626
O	-1.681798	-0.367366	1.032932
H	-3.885934	-0.934435	0.625184
H	0.471689	0.594612	2.866154
H	-1.037916	-0.150084	1.987501

IM-5

O	-1.897163	0.412725	-0.925522
O	0.393339	1.968624	-0.123416
Si	-2.382101	1.626456	-1.942560
H	-1.375894	1.902637	-3.004581
H	-3.641674	1.177224	-2.594215
H	-2.654976	2.893534	-1.212042
Si	1.624565	2.892754	0.438553
H	2.967701	2.355866	0.049354
H	1.512267	4.267588	-0.106902
H	1.619354	2.967421	1.933971
O	-1.202221	-1.469325	1.138470
Si	-2.576245	-2.318316	0.753802
H	-2.542695	-2.832438	-0.641184
H	-2.638092	-3.481956	1.681849
H	-3.810244	-1.510649	0.942915
O	-0.760502	0.861752	2.361980
SN	-0.305558	0.106412	0.232929
C	1.784142	-1.604833	-1.039156
O	0.702721	-1.103663	-1.391633
C	2.378011	-1.224810	0.345520
H	2.641478	-2.151380	0.879288
O	3.623425	-0.575243	0.045240
C	2.530212	-2.544718	-1.926274
H	2.446540	-3.551297	-1.496014
H	2.112134	-2.547304	-2.932936
H	3.590837	-2.282677	-1.931067
O	1.525027	-0.438914	1.062682
H	3.439412	0.380505	0.065798
H	-0.944328	0.004109	2.791268
H	-0.002173	1.274196	2.807963

TS-4

O	2.081668	-0.113039	0.787023
O	0.126423	2.007562	0.174067
Si	3.073566	0.909785	1.625463
H	2.403939	1.486030	2.823556
H	4.250746	0.120285	2.076564
H	3.558405	2.033048	0.776564
Si	-0.662234	3.256155	-0.536719

H	-2.105872	3.319514	-0.179846
H	-0.013917	4.538186	-0.163557
H	-0.596115	3.138259	-2.036743
O	0.528690	-1.735833	-1.096665
Si	1.561109	-3.011022	-0.851088
H	1.584666	-3.453144	0.567840
H	1.065890	-4.139057	-1.688967
H	2.949204	-2.692486	-1.281100
O	0.914876	0.651009	-2.271863
SN	0.319796	0.025681	-0.122868
C	-2.142039	-0.853487	1.176886
O	-0.877440	-0.746349	1.465909
C	-2.562098	-0.454166	-0.145699
H	-2.360075	-1.778896	0.059639
O	-3.897581	-0.299305	-0.397331
C	-3.109444	-1.277300	2.247357
H	-4.086684	-1.527098	1.834399
H	-2.700765	-2.122017	2.805448
H	-3.222569	-0.436232	2.939491
O	-1.701424	0.044392	-0.988092
H	-3.982079	-0.131776	-1.350220
H	0.726678	-0.157554	-2.781205
H	0.404349	1.392248	-2.641321

IM-6

O	1.692798	-1.404852	-0.528228
O	1.124918	1.002144	1.441418
Si	3.246630	-1.815025	-0.165587
H	3.416052	-2.140787	1.278543
H	3.611284	-3.012643	-0.966968
H	4.194740	-0.715485	-0.498781
Si	1.580755	2.595742	1.393800
H	0.406293	3.502446	1.279871
H	2.282024	2.889735	2.672188
H	2.504128	2.875772	0.262655
O	-0.070174	1.006017	-1.435971
Si	0.522282	1.164146	-2.969720
H	2.003247	1.304480	-2.991728
H	0.150468	0.000507	-3.822825
H	-0.079078	2.388619	-3.564652
O	0.271581	-1.395973	2.159588
SN	0.237535	-0.224422	0.118915
C	-2.590428	-0.867189	-0.433119
O	-1.363985	-1.465880	-0.112530
C	-2.722707	0.446382	0.334089

H	-2.629845	-0.576417	-1.496544
O	-3.909604	1.056627	0.262152
C	-3.750542	-1.828813	-0.138281
H	-4.709826	-1.386211	-0.417626
H	-3.595250	-2.741675	-0.716945
H	-3.773731	-2.094047	0.922874
O	-1.774618	0.923481	0.964326
H	-3.837485	1.909779	0.729820
H	-0.590612	-1.782610	2.375890
H	0.490219	-0.703244	2.807395

TS-6

O	-1.823136	-1.279535	0.422463
O	-1.186811	1.357272	-1.327581
Si	-2.762823	-2.492390	-0.193487
H	-1.969407	-3.728782	-0.432558
H	-3.821916	-2.792491	0.805453
H	-3.411105	-2.098535	-1.474172
Si	-1.675921	2.924183	-1.130855
H	-0.523182	3.825138	-0.850625
H	-2.318746	3.358927	-2.398393
H	-2.655043	3.066463	-0.019416
O	0.040701	0.835300	1.542887
Si	-0.589831	0.751359	3.073048
H	-2.039806	1.076424	3.102557
H	-0.389880	-0.594215	3.677135
H	0.141536	1.748974	3.900796
O	0.122296	-1.277620	-1.911433
SN	-0.386780	-0.060979	-0.192337
C	2.622068	-0.915093	0.321992
O	1.359269	-1.467761	0.026035
C	2.673282	0.512613	-0.218631
H	2.717525	-0.826620	1.412306
O	3.839525	1.142414	-0.065444
C	3.765605	-1.782660	-0.223313
H	4.736449	-1.363302	0.050050
H	3.675062	-2.783399	0.203800
H	3.710042	-1.864729	-1.313022
O	1.701466	1.048925	-0.756485
H	3.736086	2.055635	-0.393961
H	1.036890	-1.567153	-1.136380
H	0.322339	-0.788614	-2.722408

IM-7

O	-1.791477	-1.337343	0.307453
O	-1.363301	1.582112	-1.055445

SI	-2.642479	-2.599483	-0.330087
H	-1.765627	-3.773962	-0.598934
H	-3.677470	-3.003431	0.657945
H	-3.321570	-2.233330	-1.604511
SI	-1.885394	3.051681	-0.513425
H	-0.742372	3.961629	-0.218885
H	-2.711913	3.668600	-1.584182
H	-2.709397	2.934307	0.720495
O	0.127693	0.541501	1.527367
SI	-0.479863	0.141705	3.019025
H	-1.932990	0.422394	3.141310
H	-0.235275	-1.289412	3.348604
H	0.253613	0.974290	4.012683
O	0.066669	-0.885261	-2.083804
SN	-0.435565	-0.015207	-0.317197
C	2.739874	-0.823227	0.248371
O	1.516614	-1.480698	-0.081354
C	2.665878	0.637517	-0.202161
H	2.779167	-0.799404	1.341728
O	3.804308	1.315473	-0.021795
C	3.958570	-1.559456	-0.315141
H	4.881606	-1.068578	-0.000971
H	3.956427	-2.585953	0.057491
H	3.932661	-1.581335	-1.409344
O	1.660301	1.157482	-0.677300
H	3.643939	2.243743	-0.277157
H	-0.300458	-0.419516	-2.848068
H	1.483822	-1.679434	-1.042949
LA			
C	0.665309	0.104308	-0.392651
O	1.362200	-1.131620	-0.315314
C	-0.787814	-0.168424	-0.003793
O	-1.206295	-1.112696	0.629911
C	1.256475	1.181281	0.534911
H	1.267314	0.822959	1.567848
H	2.284268	1.408998	0.231924
H	0.673705	2.104345	0.477976
O	-1.592347	0.843405	-0.452565
H	-2.492397	0.634904	-0.144355
H	0.650313	0.484097	-1.424051
H	2.304519	-0.951001	-0.436400