A QM/MM Exploration of the Potential Energy Surface of Pyruvate to Lactate Transformation Catalyzed by LDH. Improving the Accuracy of Semiempirical Descriptions.

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Supporting Information

S.1. Geometries (in Å) and absolute energies at the HF/6-31G(d,p) level (in a.u.) of the complexes shown in figure 3.

Complex 1

scf done: -340.279934

C	-1.400763	0.023721	-0.345822
N	-1.154338	-0.079178	1.015019
C	0.145952	-0.093250	1.233277
N	0.755722	-0.004649	0.082379
C	-0.188067	0.069938	-0.923589
C	-2.783075	0.064079	-0.912285
H	-1.850198	-0.134742	1.729055
H	0.090214	0.148537	-1.951123
H	1.763080	0.006053	-0.033689
H	0.619213	-0.164930	2.188976
H	-2.733630	0.146092	-1.989123
H	-3.329993	-0.838851	-0.665360
H	-3.333466	0.917111	-0.531787
O	3.579738	0.010413	-0.054400
H	4.140307	0.776276	-0.093926
H	4.142599	-0.738988	-0.209090

Complex 2

scf done: -340.278326

C	0.161774	-0.000243	-0.925923
N	-0.035874	0.000746	0.445177
C	1.122403	-0.000643	1.058650
N	2.070884	-0.002331	0.151020
C	1.493657	-0.002149	-1.105649
C	-0.972285	0.000936	-1.899064
H	-0.935094	0.002015	0.913535
H	2.081162	-0.003346	-1.996904
H	3.049917	-0.003532	0.346011
H	1.270774	-0.000379	2.117092
H	-0.588757	0.000683	-2.909878
H	-1.591734	-0.879183	-1.769728
H	-1.590102	0.882149	-1.769447
O	-2.574798	0.004308	1.762200
H	-2.753213	0.007749	2.695072
H	-3.422930	-0.016934	1.335186

Complex 3

scf done: -530.661311

N	-1.781994	-0.108210	-0.027474
C	-1.780659	-0.117053	1.372845
C	-0.679051	-0.123817	2.099608
C	0.704144	-0.098962	1.500755
C	0.613068	-0.060682	-0.009661
C	-0.557615	-0.026990	-0.646713
H	-2.757294	-0.140218	1.819025
H	-0.770425	-0.158979	3.170314
H	1.271748	-0.970402	1.822535
C	1.894251	0.031219	-0.750077
H	-0.605514	0.070306	-1.715081
C	-2.955578	0.386838	-0.713488
H	1.266491	0.758691	1.858644
N	1.881383	-0.308336	-2.083807
O	2.901158	0.411127	-0.217495
H	2.791405	-0.343647	-2.490840
H	1.273168	-1.041104	-2.372253
H	-3.841571	-0.063071	-0.283679

H	-3.052358	1.468890	-0.652125
H	-2.911998	0.103017	-1.757221
O	-0.120079	-2.751652	-2.472909
H	-0.372808	-2.831970	-1.563463
H	0.125254	-3.625098	-2.745525

Complex 4

scf done: -415.996701

C	-0.009757	-0.105037	0.002444
C	-0.005615	-0.063410	1.551221
O	0.973920	-0.229448	-0.671836
O	0.550573	-0.996258	2.115866
O	-0.601076	0.924085	1.990480
C	-1.370940	0.082746	-0.646119
H	-1.288770	-0.002116	-1.724284
H	-2.068044	-0.662500	-0.270746
H	-1.763940	1.052907	-0.368500
H	1.007908	-0.493770	-2.617377
O	0.972295	-0.877601	-3.482721
H	1.020954	-1.813819	-3.346545

Complex 5

scf done: -416.000210

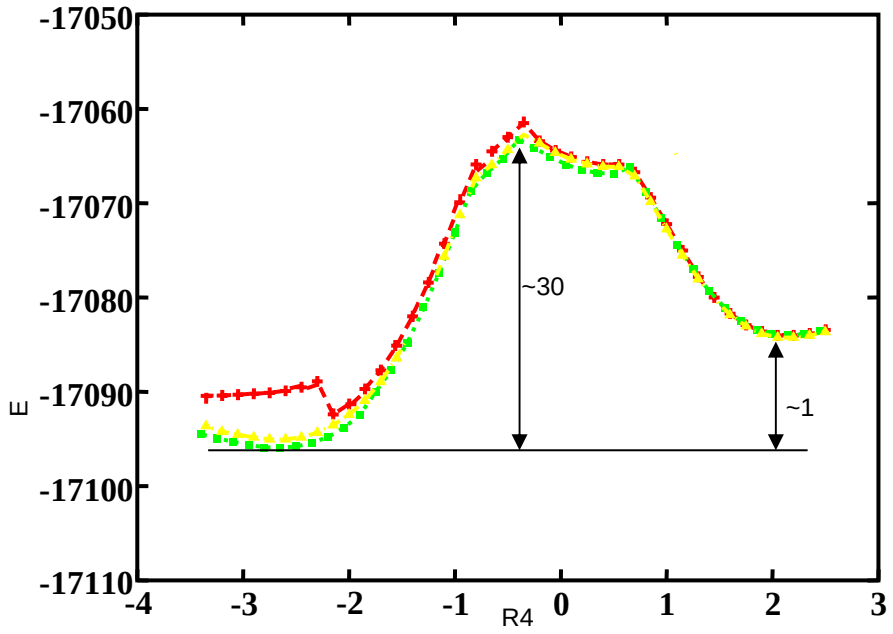
C	-1.018000	3.319000	3.777000
H	-0.162000	3.577000	4.447000
H	-1.893000	3.032000	4.410000
H	-1.285000	4.208000	3.160000
C	-0.630000	2.141000	2.932000
O	-0.626000	2.217000	1.697000
C	-0.254000	0.888000	3.735000
O	-1.186000	0.094000	4.032000
O	0.953000	0.766000	4.078000
H	1.047178	-0.951907	5.281361
O	0.501760	-1.642403	5.650744
H	-0.326991	-1.385828	5.253375

Complex 6

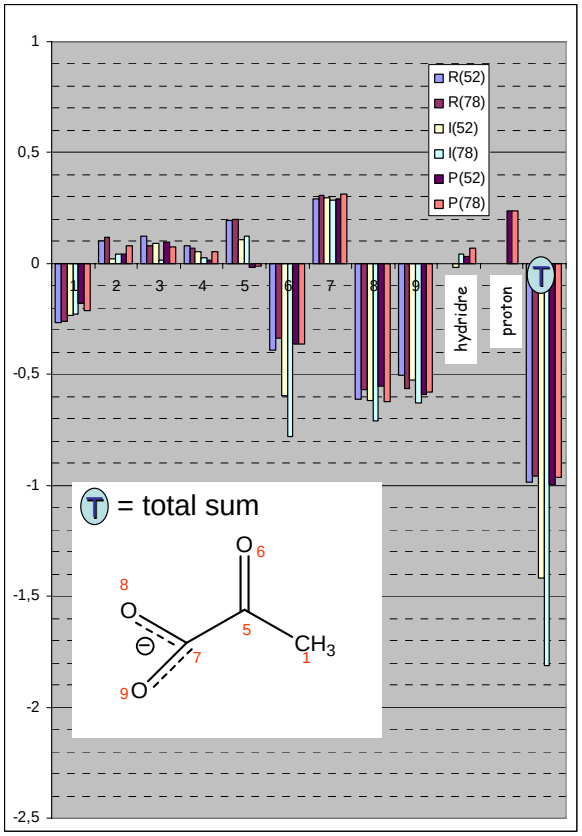
scf done: -230.095215

C	1.218333	-0.217622	0.000001
H	2.059314	0.468983	-0.000038
C	-0.092541	0.543047	0.000002
H	-0.152217	1.184134	-0.877704
H	-0.152251	1.184085	0.877742
O	-1.139031	-0.393666	-0.000001
H	-1.970873	0.058102	-0.000018
H	1.286725	-0.849271	-0.878581
H	1.286795	-0.849257	0.878585
O	-3.836176	0.832984	0.017998
H	-4.318768	0.517210	-0.733135
H	-4.302129	0.505978	0.774810

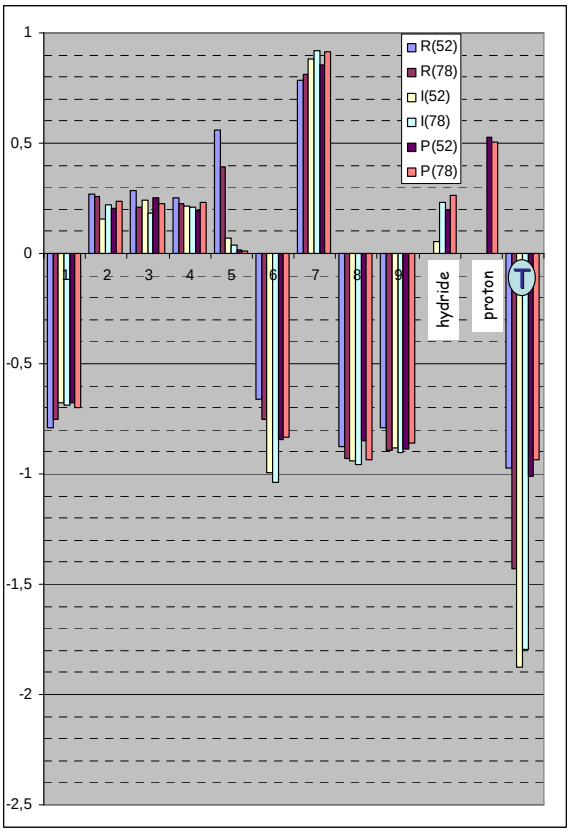
S.2. Energy profiles(kcal/mol)obtained using the $R_1+R_2=R_4$ coordinate (in Å)at the AM1/MM level with SVB correction terms. The different profiles correspond to different starting points.



S.3. Atomic charges (in a.u.) obtained for stationary structures of the HP Pathway. a) Gaussian AM1 Mulliken Charges. b) Gaussian MP2/6-31G* NPA Charges[27,28] R, I and P mean reactant, intermediate and products. The number of atoms in the QM system appears in brackets. Note that the intermediate structure is not stationary on the AM1(78)/MM PES but it is included for comparative purposes.



a)



b)