CC/DFT Route toward Accurate Structures and Spectroscopic Features for Observed and Elusive Conformers of Flexible Molecules: Pyruvic Acid as a Case Study

Supporting Information

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Table 1. The cartesian coordinates of the structures of the five stationary points optimized at the B2PLYP/aug-cc-pVTZ level of theory.

Tc-PA

O	1.070967407040	-1.331253027606	0.000000000000
C	0.761215331756	-0.156013942316	0.000000000000
C	-0.744328004242	0.190886857754	0.000000000000
C	1.718616518884	0.987150382621	0.000000000000
O	-1.157541217567	1.320331636820	0.000000000000
O	-1.523057065864	-0.893456916874	0.000000000000
H	-0.926349059715	-1.664325362788	0.000000000000
H	2.738493571933	0.617976541306	0.000000000000
H	1.534759303140	1.615216271070	-0.871424563342
H	1.534759303140	1.615216271070	0.871424563342

Tt-PA

O	1.140162516864	-1.328315129287	0.000000000000
C	0.775489039759	-0.177583653969	0.000000000000
C	-0.730161619940	0.164251990580	0.000000000000
C	1.688193041355	1.011907687533	0.000000000000
O	-1.144344908004	1.298811777464	0.000000000000
O	-1.502581832324	-0.928622639832	0.000000000000
H	-2.422458215548	-0.624452795716	0.000000000000
H	2.719103383323	0.674526377272	0.000000000000
H	1.488032677065	1.633103778496	-0.872488199756
H	1.488032677065	1.633103778496	0.872488199756

Ct-PA

O	1.286280846761	-1.250209344567	0.000000000000
C	0.787567505959	-0.152644800337	0.000000000000
C	-0.760889817379	-0.062249717138	0.000000000000
C	1.565993224156	1.131177052749	0.000000000000
O	-1.492894402192	-1.012111273474	0.000000000000
O	-1.182622382225	1.224191500931	0.000000000000
H	-2.151584176511	1.204992036778	0.000000000000
H	2.627445928310	0.906089537476	0.000000000000
H	1.304330514059	1.727380843229	-0.873732089277
H	1.304330514059	1.727380843229	0.873732089277

TS(c-t)

O	1.0928183045251	-1.3112546720169	0.2934174745585
C	0.7693000571666	-0.1814957352498	0.0065936755728
C	-0.7288188570520	0.1869036395149	0.0125118649102
C	1.7217516604637	0.9376762907824	-0.2847528282238
O	-1.1057249371338	1.2877100313340	0.3041921417264
O	-1.5574279247139	-0.8313318780394	-0.3556758787880
H	-1.8831672714310	-1.3297551340760	0.4019203672960
H	2.7418994030819	0.5708923215366	-0.2419756249519
H	1.5095801928047	1.3546011333113	-1.2699497186424
H	1.5714319048570	1.7426304611242	0.4333577390551

TS(C-T)

O	-0.0015809828	0.0189447980	1.0019925929
C	1.2065025521	-0.0045219910	1.0003121612
C	1.9444204981	-0.0036625416	-0.3448683101
C	2.0688613052	-0.0039842126	2.2283438369
O	1.9990146926	0.9428215105	-1.0843932959
O	2.5225642063	-1.1989915446	-0.5829077459
H	2.9494148608	-1.1471125315	-1.4527236740
H	1.4455832819	0.0419226184	3.1159056243
H	2.6840568128	-0.9038918145	2.2428582813
H	2.7458504391	0.8510826060	2.1991591847

Table 2. The structures of the of the T c, T t and Ct conformers evaluated by means of the "best CC" and "best cheap" composite schemes.

Pyruvic Ac. Tc
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X
O 1 one
C 2 rCO1* 1 pi2
C 3 rCOCO* 2 alpha* 1 zero
C 3 rCOCH* 2 beta* 1 pi
O 4 rCO2* 3 aCCO* 2 pi
X 6 one 4 pi2 3 zero
O 4 rCOH* 6 aOCO* 7 pi
H 8 rOH* 4 aCOH* 3 zero
H 5 rCH1* 3 aH1CC* 2 zero
H 5 rCH2* 3 aH2CC* 2 xi2*
H 5 rCH2* 3 aH2CC* 2 xi2m*

one = 1.000000000000000
pi2 = 90.000000000000000
zero = 0.000000000000000
pi = 180.000000000000000

Best	"cheap" [MP2/CBS+MP2/CV+MP2/aug+(T)]	"best" [CCSD(T)/CBS(T,Q)+CV(CT)]
rCO1	1.2109173	1.2114261171
rCOCO	1.5409483	1.5386578019
alpha	117.68538	117.6982865869
rCOCH	1.4893771	1.4893212674
beta	125.47052	125.3944374315
rCO2	1.1982884	1.1979466357
aCCO	122.71308	122.8026571870
rCOH	1.3295819	1.3296694374
aOCO	124.09936	124.3848487787
rOH	0.97094103	0.9706455610
aCOH	107.22391	106.4001738090
rCH1	1.0846851	1.0845306115
aH1CC	109.82164	109.8824438324
rCH2	1.0896050	1.0892594434
aH2CC	109.28370	109.3480729825

xi2 | 121.89281 | 121.9246122157
xi2m | -121.89281 | -121.9246122157

Pyruvic Ac. Tt
==========

X
O 1 one
C 2 rCO1* 1 pi2
C 3 rCOCO* 2 alpha* 1 zero
C 3 rCOCH* 2 beta* 1 pi
O 4 rCO2* 3 aCCO* 2 pi
X 6 one 4 pi2 3 zero
O 4 rCOH* 6 aOCO* 7 pi
H 8 rOH* 4 aCOH* 3 pi
H 5 rCH1* 3 aH1CC* 2 zero
H 5 rCH2* 3 aH2CC* 2 xi2*
H 5 rCH2* 3 aH2CC* 2 xi2m*

one = 1.000000000000000
pi2 = 90.000000000000000
zero = 0.000000000000000
pi = 180.000000000000000

Best "cheap" [MP2/CBS+MP2/CV+MP2/aug+(T)] "best" [CCSD(T)/CBS(T,Q)+CV(CT)]
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rCO1 | 1.2040073 | 1.2039464866
rCOCO | 1.5391677 | 1.5369919692
alpha | 120.18479 | 120.2925607578
rCOCH | 1.4966201 | 1.4969369208
beta | 124.98499 | 124.9735563422
rCO2 | 1.2035347 | 1.2031587388
aCCO | 122.44731 | 122.5805756248
rCOH | 1.3320848 | 1.3323916560
aOCO | 124.89198 | 124.7628184012
rOH | 0.96563396 | 0.9651064815
aCOH | 107.11810 | 106.5935392756
rCH1 | 1.0847486 | 1.0846333264
aH1CC | 109.19083 | 109.2331515100
rCH2 | 1.0894715 | 1.0891189471
aH2CC | 109.71480 | 109.7953359433
xi2 | 121.53926 | 121.5613229246
xi2m | -121.53926 | -121.5613229246

Pyruvic Ac. Ct
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X
O 1 one
C 2 rCO1* 1 pi2
C 3 rCOCO* 2 alpha* 1 zero
C 3 rCOCH* 2 beta* 1 pi
O 4 rCO2* 3 aCCO* 2 zero
X 6 one 4 pi2 3 zero
O 4 rCOH* 6 aOCO* 7 pi

H 8 rOH* 4 aCOH* 3 pi
H 5 rCH1* 3 aH1CC* 2 zero
H 5 rCH2* 3 aH2CC* 2 xi2*
H 5 rCH2* 3 aH2CC* 2 xi2m*

one = 1.000000000000000
pi2 = 90.000000000000000
zero = 0.000000000000000
pi = 180.000000000000000

Best	"cheap" [MP2/CBS+MP2/CV+MP2/aug+(T)]	"best" [CCSD(T)/CBS(T,Q)+CV(CT)]
rCO1	1.2023597	1.202549165569725
rCOCO	1.5461938	1.543671337623149
alpha	117.75383	117.805215653354594
rCOCH	1.4988816	1.499003598818730
beta	124.40465	124.369390090869089
rCO2	1.1945796	1.194824015290882
aCCO	124.31445	124.236557370703551
rCOH	1.3479471	1.347493048469949
aOCO	124.41403	124.298257447734755
rOH	0.96600811	0.965326525960292
aCOH	107.08491	106.683324816280873
rCH1	1.0850282	1.084904117127387
aH1CC	109.08072	109.076496606742481
rCH2	1.0895139	1.089207402819697
aH2CC	109.90211	109.983274426301961
xi2	121.31221	121.327308263448600
xi2m	-121.31221	-121.327308263448657