

Specificity of internal rotation in aldehydes with three-membered rings

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The equilibrium geometric parameters (XYZ coordinates) in A, and absolute energies in Hartree of PES minima obtained by MP2/cc-pVTZ

CP1CA cis

Energy: -229.490040950591

C	0.8794690266	0.0000009304	1.2096104517
C	-0.5143380054	-0.0000020303	1.7865072124
C	-0.0907138596	0.0000020178	0.3366355465
C	-0.5129986119	0.0000025346	-1.0649536483
H	1.9307057953	0.0000017550	1.4285952207
H	-0.8990083118	0.9137142351	2.2257243375
H	-0.8990099825	-0.9137285868	2.2257019917
O	0.2715968078	-0.0000022890	-1.9952919281
H	-1.6008147373	0.0000077886	-1.2319937593

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CP1CA trans

Energy: -229.492043114982

C	0.6404641412	0.0000008375	1.5738777154
C	-0.8599945783	-0.0000005438	1.4128508971
C	0.1980901223	0.0000002552	0.3438326578
C	0.4911727443	-0.0000010998	-1.0837361746
H	1.4582982063	0.0000016773	2.2704176838
H	-1.4083952510	0.9142588051	1.6077669381
H	-1.4083907062	-0.9142637745	1.6077624934
O	-0.3655798703	0.0000008761	-1.9481875049
H	1.5639586781	-0.0000040508	-1.3356852542

CP2CA cis

Energy: -229.493962810425

C	0.2915347475	0.6455448546	1.2955088691
C	0.2915346250	-0.6455448835	1.2955089032
C	-0.7426237277	0.0000000921	0.3956777003
C	-0.4980567099	0.0000000484	-1.0709810329
H	0.6885279104	1.5944503471	1.5991570781
H	0.6885267217	-1.5944507346	1.5991573541
H	-1.7862668090	0.0000002129	0.6938001785
O	0.6080208240	-0.0000000817	-1.5761241176
H	-1.4057786636	0.0000001422	-1.7021091811

CP2CA trans

Energy: -229.495737704399

C	0.6465148620	-0.0892943717	1.5470681380
C	-0.6465238719	-0.0892447558	1.5470664765
C	0.0000177657	0.4735897538	0.2938197403
C	-0.0000131599	-0.3595477398	-0.9292225310
H	1.5900196728	-0.2677816232	2.0258303424
H	-1.5900373353	-0.2678041320	2.0257853382
H	0.0000586553	1.5439396574	0.1160148464
O	0.0000041923	0.0762770721	-2.0625370259
H	-0.0000550585	-1.4505553806	-0.7274188513