

Supporting Information: Different Photoisomerization Route Found in the Structural Isomers of Hydroxy methylcinnamate

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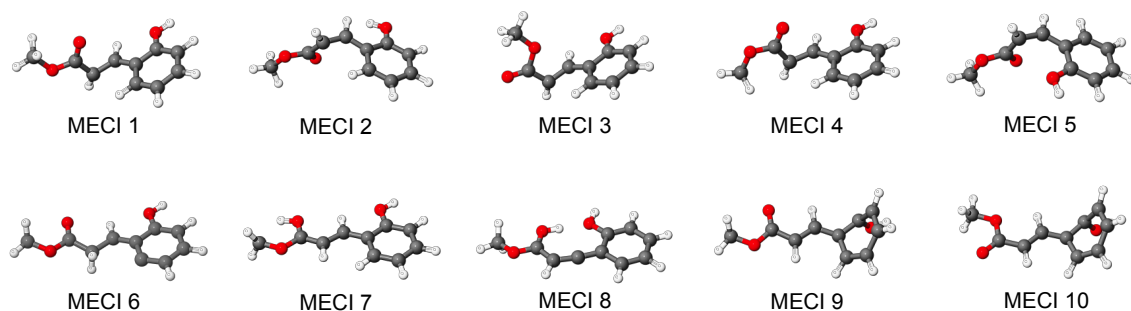
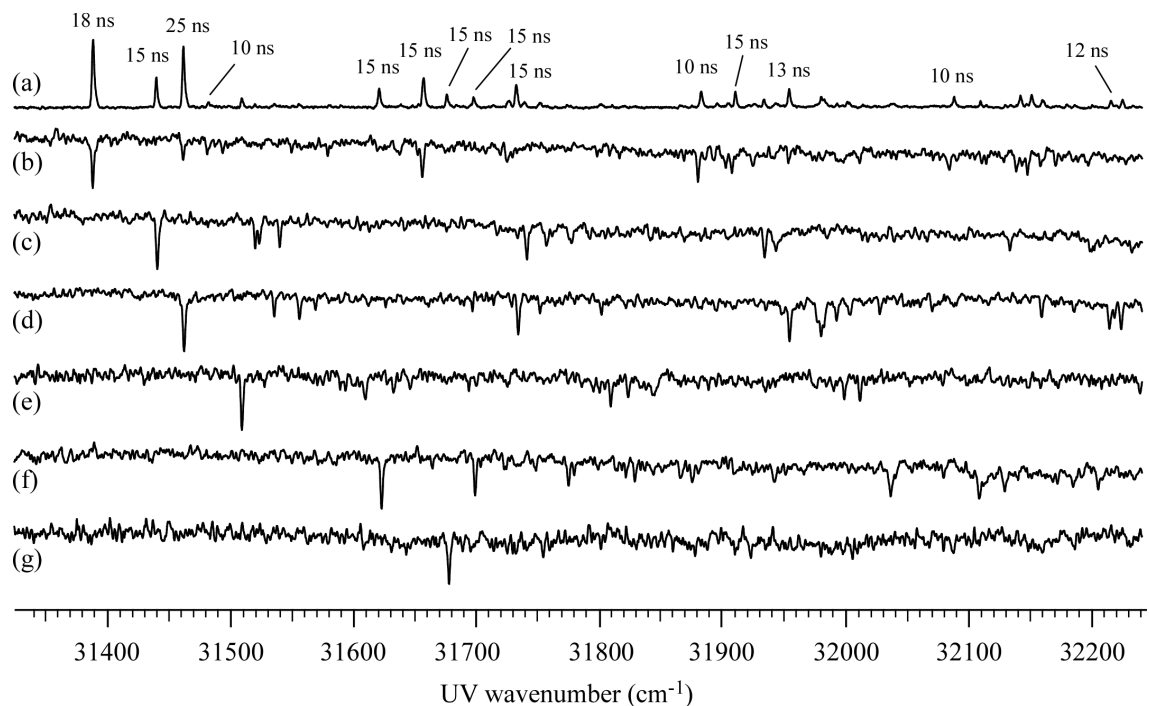


Figure S1. Ten low-lying MECIs of *trans-o*-HMC optimized at the Spin-flip TD-BHandHLYP/6-311G(*d,p*) level of theory.

conformer	aTC	sTC	aTT	sTT
B3LYP/6-311++G(d, p)	0	14	327	327
PBE0/cc-pVDZ	0	29	361	369
M05-2X/6-31+G(d)	0	40	304	312

Figure. S2. Molecular structure of the *trans-p*-HMC conformers and their relative energies in cm^{-1} calculated at (top) B3LYP/6-311G(d,p), (middle), PBE0/cc-pVDZ, and (bottom) M05-2X/6-31+G(d) levels of theory. These values are correlated with zero-point vibrational energies. Two DFT calculation methods were tested for the ground state stability. The *s-cis* conformer is $\sim 300 \text{ cm}^{-1}$ more stable than the *s-trans* conformer while the *anti* and *syn* conformers are almost equal stability.



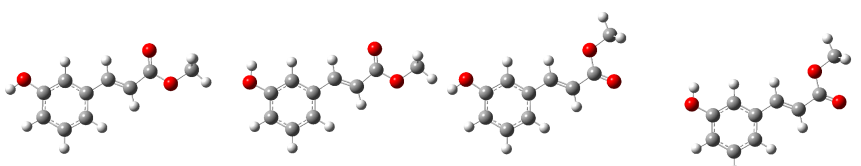
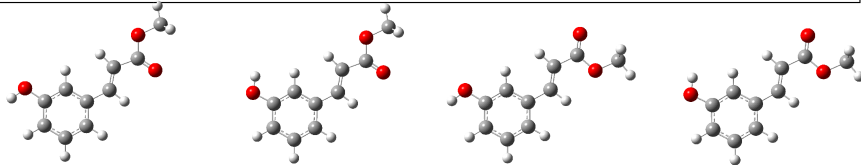
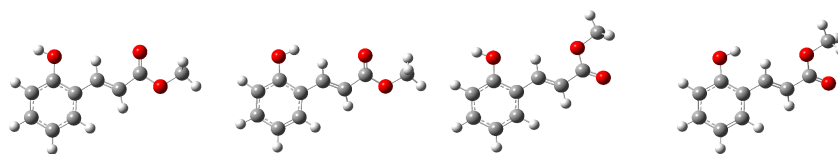
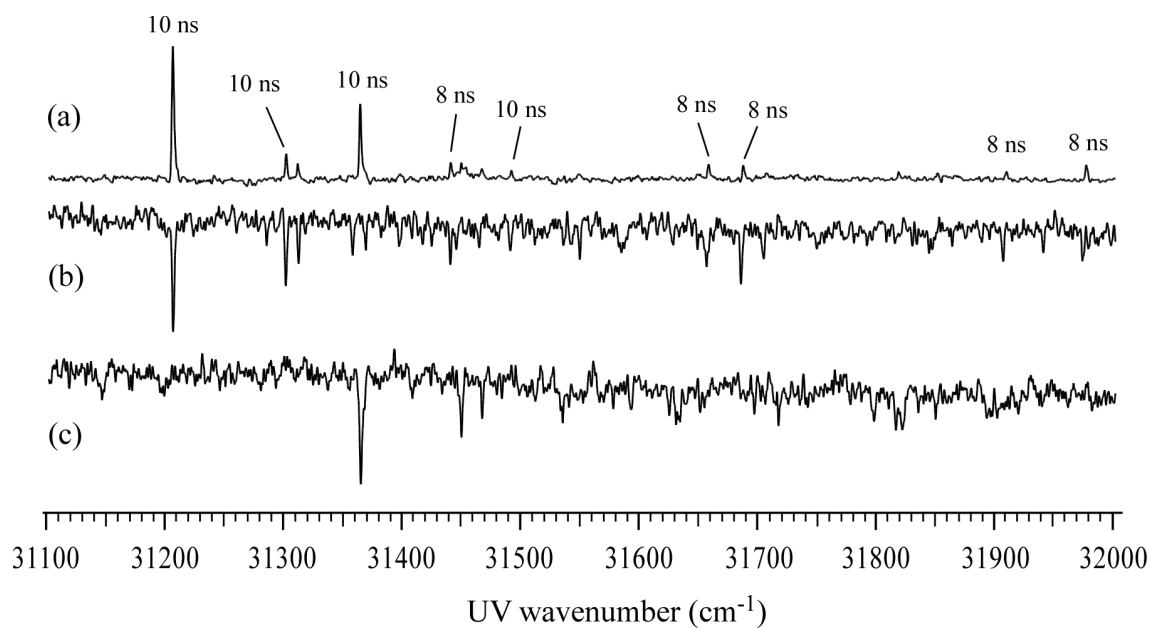
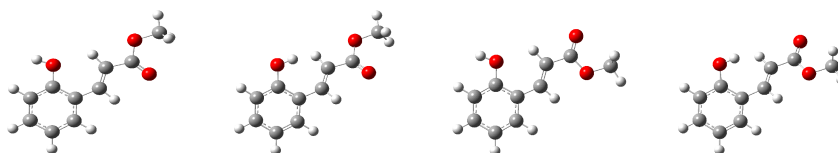
					
conformer		TTTC	CTTC	TTTT	CTTT
S_0	B3LYP/6-311++G(d, p)	30	0	310	355
	PBE0/cc-pVDZ	72	11	396	387
	M05-2X/6-31+G(d)	44	13	316	355
$S_0 \rightarrow S_1$	TD-PBE0/cc-pVDZ	33234	32964	33268	32992
					
conformer		TCTC	CCTC	TCTT	CCTT
S_0	B3LYP/6-311++G(d, p)	30	10	344	271
	PBE0/cc-pVDZ	43	0	390	305
	M05-2X/6-31+G(d)	25	0	325	254
$S_0 \rightarrow S_1$	TD-PBE0/cc-pVDZ	33358	33221	33358	33220

Figure. S3 (Upper) LIF and UV-VU hole-burning spectra of jet-cooled *m*-HMC. (Lower) Structures of lowest energy eight conformers, their relative energies (cm^{-1}) and vertical transition energies (cm^{-1}) of *m*-HMC.



conformer		TTTC	CTTC	TTTT	CTIT
S_0	B3LYP/6-311++G(d, p)	4	268	246	636
	PBE0/cc-pVDZ	65	200	367	681
	M05-2X/6-31+G(d)	135	385	343	743
$S_0 \rightarrow S_1$	TD-PBE0/cc-pVDZ	33135	31852	33283	31948



conformer		TCTC	CCTC	TCTT	CCTT
S_0	B3LYP/6-311++G(d, p)	0	312	350	648
	PBE0/cc-pVDZ	0	72	403	458
	M05-2X/6-31+G(d)	0	172	367	525
$S_0 \rightarrow S_1$	TD-PBE0/cc-pVDZ	34436	32012	34478	31979

Figure. S4 (Upper) LIF and UV-VU hole-burning spectra of jet-cooled *o*-HMC. (Lower) Structures of lowest energy eight conformers, their relative energies (cm^{-1}) and vertical transition energies (cm^{-1}) of *o*-HMC.

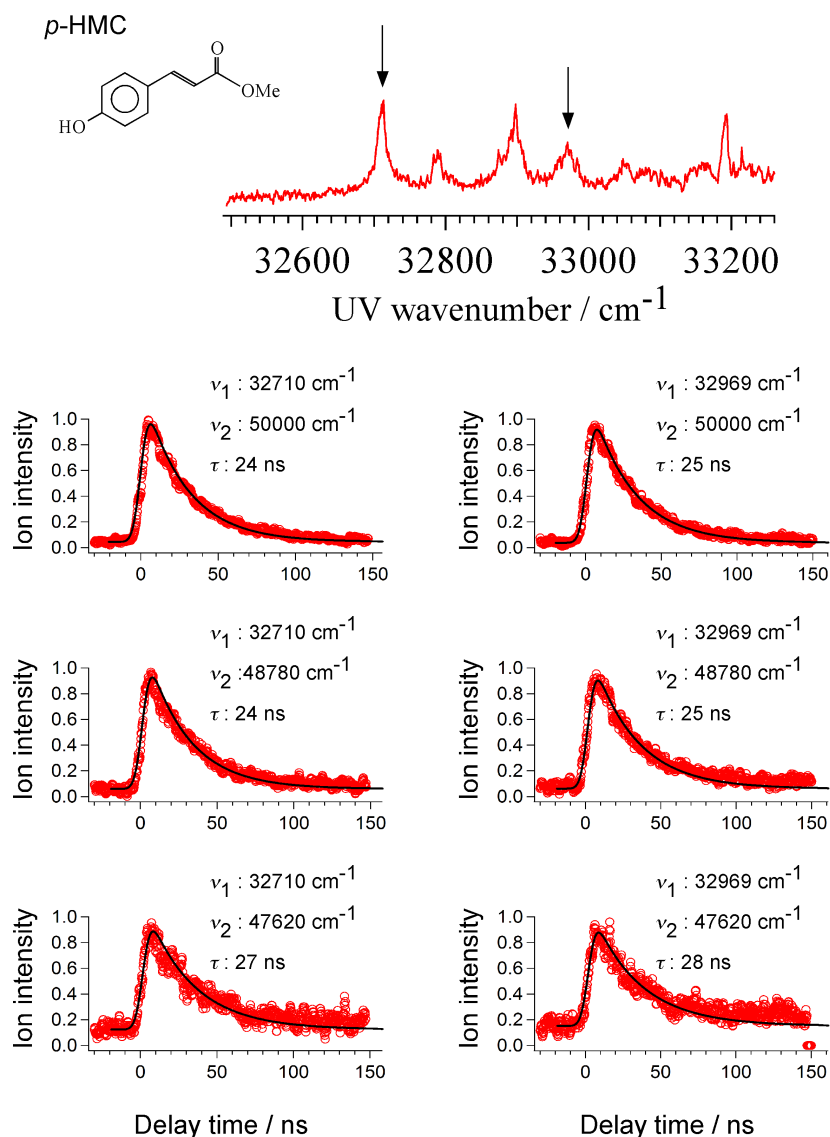


Figure. S5 Time profiles of the transient state of *p*-HMC observed by nanosecond UV-DUV pump-probe spectroscopy. Red circles are the observed ones and the black solid curves are the fitted one by convolution assuming single exponential decay. ν_1 is the pump laser frequency and ν_2 is the probe (ionization) laser frequency.

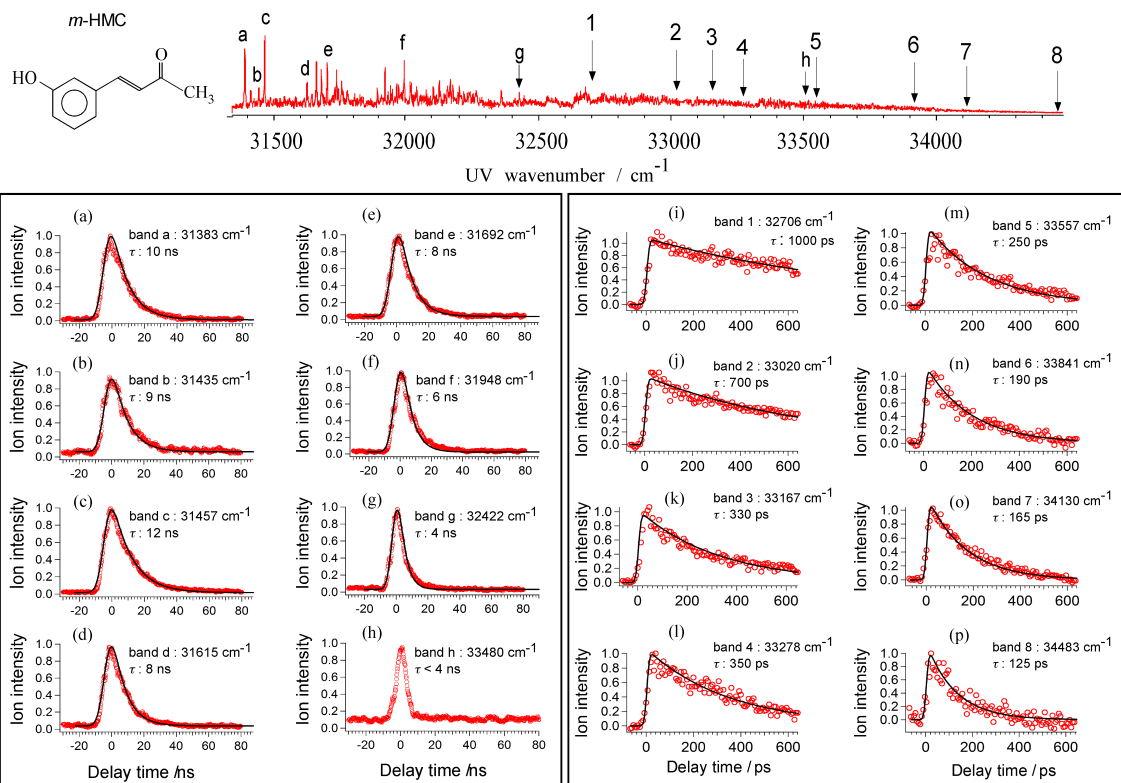


Figure S6. (Upper panel) 2C-R2PI spectrum of *m*-HMC. (Lower panel) Time profile of the vibronic bands of *m*-HMC by (a)-(h) nanosecond UV-DUV pump-probe experiment with λ_{DUV} fixed at 202 nm, and by (i)-(p) picosecond UV-UV' pump-probe experiment with $\lambda_{\text{UV'}}$ fixed at 243 nm (right). Solid curves are the fits to single exponential decay curves.

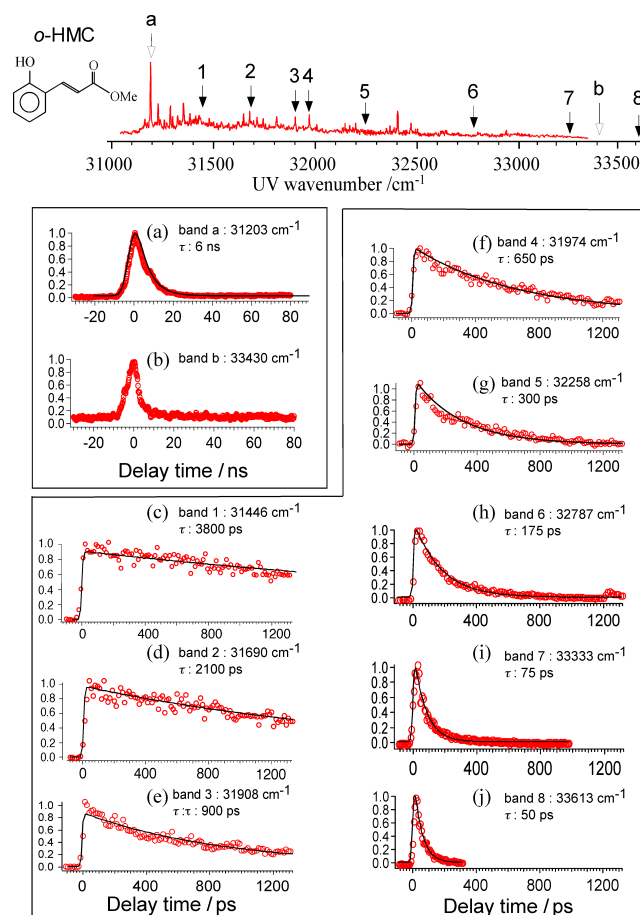


Figure S7 (Upper) 2C-R2PI spectrum of *o*-HMC. (Lower) (a), (b) Time profiles of the vibronic bands of *o*-HMC by the nanosecond UV-DUV pump-probe experiment, and (c)–(j) picosecond UV-UV' pump-probe experiment. Solid curves are the fits to single exponential decay curves.

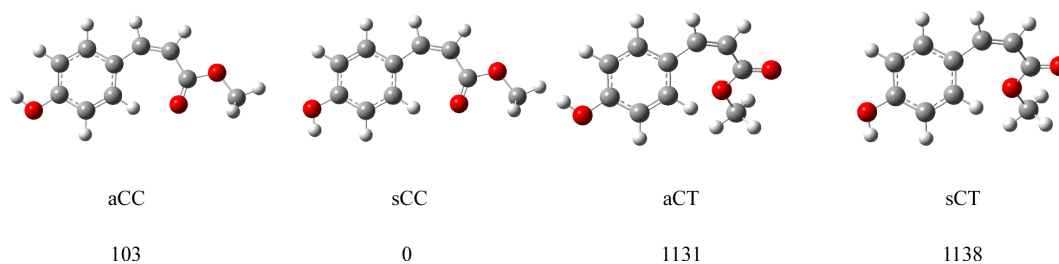


Figure S8. Molecular structure of the *cis-p*-HMC conformers and their relative energies calculated at the B3LYP/6-311G(d,p) level of theory (top) in cm^{-1} . These values are zero-point Energy corrected. aCT and sCT are the non-planar structures where the ester sp^3 orbital is interacted with aromatic C-H.

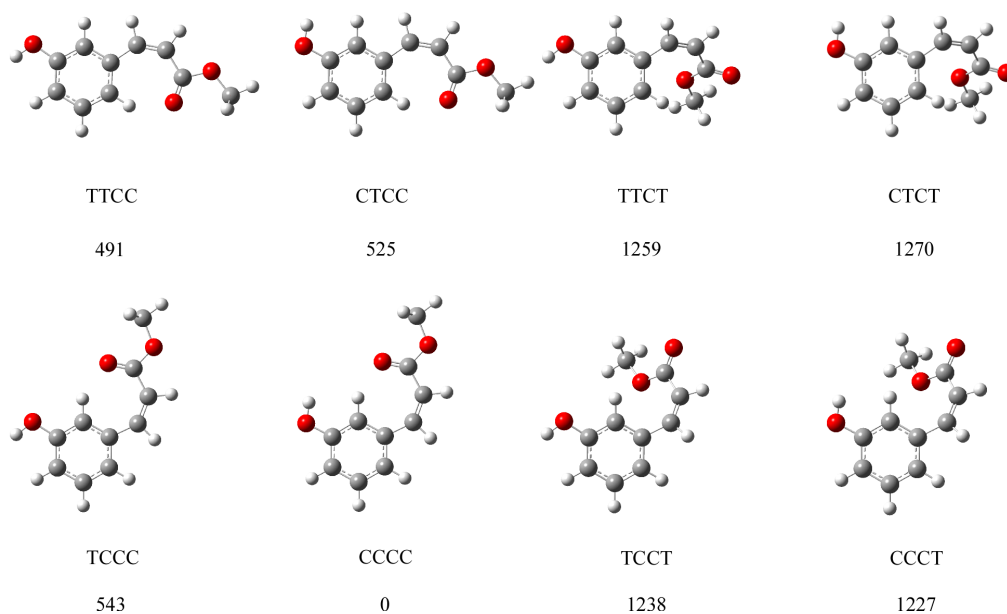


Figure. S9 Molecular structure of the *cis-m*-HMC conformers and their relative energies calculated at the B3LYP/6-311G(d,p) level of theory (top) in cm^{-1} . These values are zero-point Energy corrected.

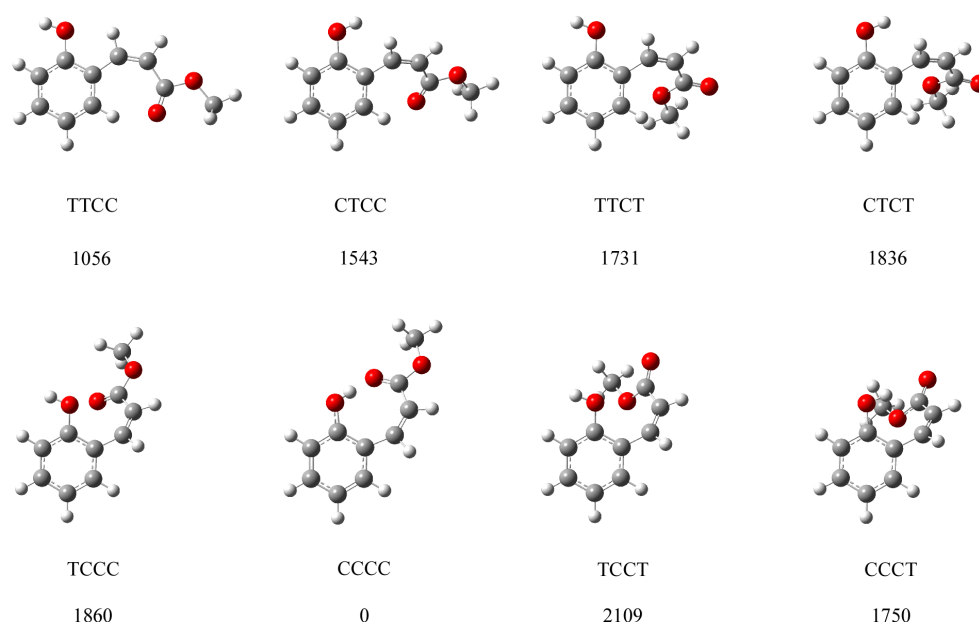


Figure S10. Molecular structure of the *cis-o*-HMC conformers and their relative energies calculated at the B3LYP/6-311G(d,p) level of theory (top) in cm^{-1} . These values are zero-point Energy corrected.

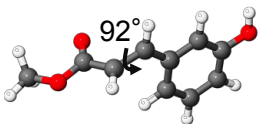
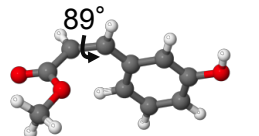
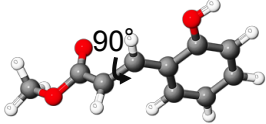
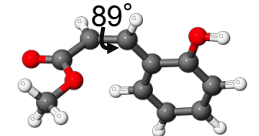
EQ	Structure	Energy / cm^{-1}
<i>m</i> -EQ 1		17789
<i>m</i> -EQ 2		17683
<i>o</i> -EQ 1		17484
<i>o</i> -EQ 2		17350

Figure S11. The optimized structures and 0-0 transition energies of the *m*-, *o*-HMC in the T_1 state. Results at the $U\omega B97XD/6-311G(d,p)$ level of theory.

Table S1. Potential Energy E of (a) *trans-m*-HMC and (b) *trans-o*-HMC at the $^1\pi\pi^*$ EQ at the TD- ω B97XD/6-311G(d,p) level of theory. The origin of the Energy is the S_0 EQ of each molecule.

(a) <i>trans-m</i> -HMC			(b) <i>trans-o</i> -HMC		
State	Character	E / cm^{-1}	State	Character	E / cm^{-1}
T ₁	$^3\pi\pi^*$	16779	T ₁	$^3\pi\pi^*$	16095
T ₂	$^3\pi\pi^*$	28111	T ₂	$^3\pi\pi^*$	30060
T ₃	$^3\pi\pi^*$	33273	T ₃	$^3\pi\pi^*$	32674
T ₄	$^3n\pi^*$	35424	T ₄	$^3n\pi^*$	35321
S ₁	$^1\pi\pi^*$	32671	S ₁	$^1\pi\pi^*$	32149
S ₂	$^1\pi\pi^*$	37904	S ₂	$^1n\pi^*$	38024
S ₃	$^1n\pi^*$	38184	S ₃	$^1\pi\pi^*$	38245

Appendix: The XYZ coordinates of the optimized structure in Å,

absolute Energy in Hartree, and lowest vibrational frequency in cm^{-1}

Computational level: Spin-flip TD-BHandHYP/6-311G(*d,p*) for S_1/S_0 MECIs and (TD-,U)ωB97XD/6-311G(*d,p*) for the others

(1) *p*-HMC

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trans-p-HMC S_0 EQ, SYMMETRY = C_s , ENERGY = -612.702543451147, Freq=29.01092721

C	2.706333765419	1.033744308635	-0.019744333214
C	1.340051698081	1.271048684256	-0.014133499086
C	0.417141648549	0.223404889771	-0.009337419636
C	0.916788311943	-1.086869302941	-0.010361152756
C	2.273581484376	-1.338096838512	-0.015878294812
C	3.179031384304	-0.275248822085	-0.020599748372
H	3.403346411179	1.866420146952	-0.023421825525
H	0.980361168060	2.294641152942	-0.013515719024
H	0.232204281918	-1.927181473067	-0.006735982357
H	2.658634531654	-2.350347851241	-0.016628546253
O	4.497685271995	-0.581445771133	-0.025852029012
C	-1.010085103064	0.537306429188	-0.003693823515
C	-2.035038854829	-0.319875825651	-0.000095940745
H	-1.267452112564	1.594657031073	-0.002528207728
H	-1.915611016508	-1.396457295481	-0.001060007090
C	-3.417782539980	0.193487345513	0.004499634189
O	-3.744398663696	1.354401319170	0.007382701083
O	-4.302044456071	-0.819643892227	0.004669586314
C	-5.674768596072	-0.434758407782	0.007346348360
H	-5.910577590937	0.156418443989	-0.879560215287
H	-5.907452977930	0.155538941770	0.895645122895
H	-6.241463126801	-1.363347316572	0.007860890841
H	5.014454966958	0.225812966439	-0.028699124265

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trans-p-HMC T_1 *p*-EQ 1, SYMMETRY = C_1 , ENERGY = -612.616830921665, Freq = 36.89538041

C	2.658246473935	0.981268963270	0.235667671426
C	1.420136536724	1.398739976669	0.677266256753
C	0.299609427741	0.532323285110	0.662484668401
C	0.508392524913	-0.782331277134	0.169137348675
C	1.744197182054	-1.198981445997	-0.269922225176
C	2.831880153058	-0.320996794082	-0.241566112628
H	3.500474379619	1.667192808987	0.256515163160
H	1.296793304260	2.412578140498	1.042519927078
H	-0.328293962716	-1.471910803884	0.135898073223
H	1.897191082278	-2.202843459657	-0.647201637768
O	4.024352653138	-0.786409234245	-0.688137696752
H	4.681398169065	-0.091439973502	-0.626556336238
C	-0.960738501570	0.972777833649	1.114569450914
C	-2.157049847831	0.141822519722	1.139120067612
H	-1.057616955440	2.000676927755	1.458311666526
H	-2.417027397738	-0.449717406192	2.013579380272

C	-3.072223069402	0.093899949227	0.007665006887
O	-2.940781361003	0.709653444081	-1.025105220301
O	-4.108373817126	-0.737795835147	0.249859361063
C	-5.058084623633	-0.846993297155	-0.806235363403
H	-4.583795766890	-1.222094707794	-1.715481018017
H	-5.509318319742	0.123757026697	-1.021703463800
H	-5.812430474692	-1.547219108877	-0.453797592929

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trans-p-HMC T_1 *p*-EQ 2, SYMMETRY = C_1 , ENERGY = -612.617353351549, Freq = 31.52602251

C	2.426732775238	0.750934198322	-0.757105969394
C	1.211232958930	0.566217686851	-1.382597684716
C	0.214578809006	-0.273010070467	-0.827575377248
C	0.521126491134	-0.910427176393	0.403156764241
C	1.734523013262	-0.727092748415	1.026209053343
C	2.699811373068	0.105816590200	0.452381125496
H	3.173465446438	1.400540909085	-1.205103087941
H	1.010412740705	1.073197130456	-2.320301266370
H	-0.219447893033	-1.557517679244	0.860951378409
H	1.963022274227	-1.216431351826	1.965291020498
O	3.875413863480	0.249228996785	1.112254468923
H	4.447546549873	0.840376483702	0.620650455772
C	-1.025374051633	-0.449873230953	-1.475893543611
C	-2.094662137347	-1.305581138251	-0.978556643095
H	-1.205680715873	0.090563562286	-2.403278279468
H	-2.179100957202	-2.343865328846	-1.288771967622
C	-3.137686464504	-0.867742370373	-0.061750235876
O	-4.027152974073	-1.583169563057	0.344358074965
O	-3.002547473337	0.423229012801	0.294843433327
C	-3.983955855391	0.910282878865	1.205219218582
H	-3.960616719036	0.342754453747	2.137691047668
H	-4.983786370200	0.834733755896	0.772882163438
H	-3.725024496728	1.950989503835	1.387242173671

(2) *m*-HMC

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trans-m-HMC CTTC S_0 EQ, SYMMETRY = C_s , ENERGY = -612.701368561282, Freq = 16.13773991

C	2.710764594533	0.993915329358	0.000065661680
C	1.342335710934	1.243255772361	0.000045224458
C	0.422119210081	0.191459228782	0.000026396039
C	0.897173697476	-1.122634664395	0.000030037923
C	2.262973180854	-1.363797487066	0.000046369645
C	3.174989673001	-0.318054689243	0.000064748366
O	3.635314788142	1.986793028863	0.000083210005
H	0.979279906472	2.267827560308	0.000042216881

H	0.205844752789	-1.956029249229	0.000005027297
H	2.627599315399	-2.384612356291	0.000045877277
H	4.243103645259	-0.496924979374	0.000083284977
C	-1.005645935216	0.525961107110	0.000001111611
C	-2.035725204660	-0.322318280300	0.000051401643
H	-1.252379278482	1.585619919122	-0.000048691272
H	-1.924102951169	-1.399587245549	0.000118416938
C	-3.416655759818	0.203130268203	0.000025598698
O	-3.730677172365	1.366938292699	-0.000057601258
O	-4.307351820479	-0.802095913323	0.000097685810
C	-5.678118538089	-0.407636615142	0.000058235776
H	-5.907417559424	0.184499322006	-0.887777400662
H	-5.907401969229	0.184606579471	0.887829374839
H	-6.250749783611	-1.332406719020	0.000139842105
H	3.192517754602	2.836675967656	0.000075852224

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trans-m-HMC S₀ CTTC EQ, Spin-Flip TD-BHandHLYP/6-311G (d,p), SYMMETRY = C_s, ENERGY = -612.552274791300

C	2.704181259124	0.984548449844	0.000065613918
C	1.341207721045	1.238954213635	0.000035959657
C	0.419722054296	0.196784146876	0.000029958166
C	0.885851338278	-1.112120234937	0.000018423167
C	2.245307508962	-1.357574386667	0.000039449517
C	3.158834693634	-0.320020832402	0.000074682556
O	3.625638275032	1.974316929454	0.000088933354
H	0.987174356121	2.258027884012	0.000042534503
H	0.196190382603	-1.936233932414	0.000002744841
H	2.603101019861	-2.372739747835	0.000044589347
H	4.218474631285	-0.503218454573	0.000082207676
C	-1.002409841874	0.538742771780	0.000010470733
C	-2.035645002415	-0.308594845925	0.000036218365
H	-1.242014374591	1.590438196239	-0.000036484492
H	-1.922755980668	-1.376954688823	0.000094859284
C	-3.409203697891	0.205751615997	0.000025385223
O	-3.725614272189	1.360622679709	-0.000031529160
O	-4.292841549416	-0.794210874986	0.000087922380
C	-5.661081030041	-0.417377524934	0.000056173897
H	-5.895558655970	0.167353015456	-0.881468985276
H	-5.895503863790	0.167557010947	0.881463005945
H	-6.220522289771	-1.341475652924	0.000199312450
H	3.195257575371	2.822008439495	0.000090434936

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trans-m-HMC CTTC ¹ππ* EQ, SYMMETRY = C_s, ENERGY = -612.546438773380, Freq = 38.69046659

C	2.720967550950	1.024446775273	0.000019689601
C	1.372489939417	1.373991309521	0.000003152307
C	0.377285747924	0.381615669705	0.000022074902
C	0.846938148376	-1.001555357580	0.000047141438
C	2.200862667878	-1.322060626998	0.000064467679
C	3.165051153823	-0.331104725695	0.000052482204
O	3.691576120743	1.938683195874	0.000003951497
H	1.086429764243	2.421268937664	-0.000023526184
H	0.116185810762	-1.799586949804	0.000058930190
H	2.497280234864	-2.364173522747	0.000088158957
H	4.226782033303	-0.536484187990	0.000062626535

C	-0.999599681922	0.685564130578	0.000023405215
C	-2.022668826941	-0.253557790491	0.000025219092
H	-1.295051573610	1.729898173807	0.000015120611
H	-1.850012352730	-1.322021015853	0.000016308874
C	-3.399388747197	0.182852454429	0.000024601077
O	-3.788381547289	1.336417409617	0.000040246821
O	-4.257781442025	-0.872275624235	0.000006448573
C	-5.635034110597	-0.528275042232	0.000010763861
H	-5.892510946852	0.056787367555	-0.886327954975
H	-5.892531776213	0.056809093742	0.886326181141
H	-6.177812232836	-1.472291711784	-0.000004211969
H	3.312517467933	2.822673189637	-0.000014615451

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m-HMC *trans* → *cis* ¹ππ* TS 1, ENERGY = -612.541377185724, SYMMETRY = C₁, Freq = -214.87798663

C	-2.674520832	1.024470664	-0.097837989
C	-1.380266996	1.398562883	-0.386436954
C	-0.354361002	0.422997199	-0.459992445
C	-0.708527342	-0.952460690	-0.236850562
C	-2.011015486	-1.296686808	0.079737821
C	-3.001326371	-0.330105403	0.142311893
O	-3.699756815	1.898970386	-0.022219944
H	-1.130830087	2.443005252	-0.549353578
H	0.060204543	-1.710188195	-0.339027774
H	-2.265077192	-2.334895642	0.258964064
H	-4.033797341	-0.581242475	0.352120244
C	0.987462193	0.766381392	-0.691210860
C	2.044977000	-0.181230844	-0.652190867
H	1.244753129	1.822712225	-0.773269779
H	2.011323441	-1.113765634	-1.210883646
C	3.271407628	0.136093760	0.037534561
O	3.501261932	1.177960887	0.626174537
O	4.180546948	-0.867402590	-0.064023876
C	5.423940156	-0.619959706	0.577747360
H	5.907879827	0.266481135	0.160829465
H	5.285027136	-0.466692862	1.650780829
H	6.031840873	-1.504782141	0.396750729
H	-3.377818598	2.788935715	-0.179566524

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trans-m-HMC ¹ππ*/¹ππ* MECI 2, ENERGY = -612.538716933752, SYMMETRY = C₁

C	3.328559216215	-0.497953311620	-0.108199667097
C	2.004060469861	-0.911121220290	-0.174073814733
C	0.950127398716	0.009908744969	-0.033209785092
C	1.301415612325	1.376359748243	0.173433176158
C	2.629998891818	1.770668983400	0.236390298730
C	3.659249992259	0.851879531543	0.099989326076
O	4.360288309116	-1.359139973594	-0.237524211209
H	1.775051549403	-1.961131584861	-0.335052251063
H	0.523213266876	2.121212480912	0.282766782031
H	2.866122396705	2.816562994277	0.396430593097
H	4.701821221738	1.138002627383	0.149389294244
C	-0.405630424024	-0.434529333666	-0.095857080726
C	-1.525643800204	0.379579313802	0.038126087420
H	-0.567216563571	-1.494704448738	-0.257589746105

H	-1.465359134482	1.448882100076	0.202165523548
C	-2.825428445727	-0.135442695463	-0.025882160378
O	-3.102228532164	-1.360392982467	-0.206987571108
O	-3.844827547000	0.731749004279	0.115090681954
C	-5.169061733074	0.204184139886	0.046961334129
H	-5.825730691269	1.061236937201	0.176504420905
H	-5.340681208438	-0.523964079139	0.842782134761
H	-5.351968578881	-0.266971185961	-0.921350579244
H	4.020627538016	-2.246055448742	-0.373856592258

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m-HMC *trans*→ *cis* S₀ TS 2, ENERGY = -612.617009155986, SYMMETRY = C₁, Freq = -762.07675574

C	3.410088743132	0.464023759384	-0.159574802859
C	2.245593202909	0.947618515971	0.407332957198
C	1.069605687182	0.158554881442	0.433375304328
C	1.119854861536	-1.134624952971	-0.138276875483
C	2.294567510837	-1.601839490542	-0.698335175089
C	3.443354331792	-0.818961149333	-0.716592749444
O	4.559956884428	1.185578974037	-0.207841552653
H	2.222198411830	1.945388524199	0.837641072028
H	0.230308818668	-1.754057777575	-0.135745306201
H	2.323530727540	-2.593892918976	-1.134684619091
H	4.367128199877	-1.175252545206	-1.154993730147
C	-0.113546454619	0.667252491454	1.017009819828
C	-1.366596924334	-0.070171300998	1.102212763078
H	-0.094538050994	1.675752927907	1.427730439299
H	-1.603857342244	-0.682965903940	1.968877202949
C	-2.366808838185	0.010979450238	0.045679134286
O	-2.265433896477	0.673225140102	-0.961064266982
O	-3.440957056607	-0.755296003494	0.327877796553
C	-4.473697192896	-0.737724753651	-0.654031103900
H	-4.098663634831	-1.095638150664	-1.615004981498
H	-4.864598128705	0.273407159689	-0.784941683813
H	-5.250232831599	-1.400179671913	-0.277637067701
H	4.412030144459	2.045855525996	0.187492178448

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m-HMC S_i/S₀ MECI 1, Spin-Flip-TD-BHLYP/6-311G(*d,p*), ENNERGY = -612.424307954517

C	3.206648698184	0.570747698877	-0.302800710214
C	2.020807380313	0.929412245021	0.284236939706
C	0.997031441157	-0.026567559615	0.455721739734
C	1.194330794353	-1.347426105902	0.022823582720
C	2.392775167027	-1.694361900795	-0.559126368057
C	3.389957167061	-0.748869441879	-0.721635787219
O	4.234215020139	1.420297118593	-0.506371899133
H	1.852854454917	1.941880907803	0.613335177884
H	0.396589857903	-2.050397252935	0.161620156182
H	2.561632119884	-2.701879520582	-0.894662539154
H	4.330164162715	-1.007690378501	-1.176021042676
C	-0.208836456197	0.356455550152	1.067192373914
C	-1.357588954771	-0.471765924257	1.299343258242
H	-0.204649218354	1.394298184615	1.400146225159
H	-1.607485459477	-0.877927896124	2.258544895834
C	-2.229537211908	-0.193007550064	0.274123908669
O	-1.872035819659	0.556012361667	-0.657719319753

O	-3.465208796522	-0.730130418642	0.301661291439
C	-4.299628847062	-0.403912642301	-0.788638376087
H	-3.918677666983	-0.822413496036	-1.714526390927
H	-4.389713535792	0.669464717810	-0.909001814426
H	-5.265390141106	-0.835557760635	-0.560666283431
H	4.001033016867	2.300371794899	-0.231074265278

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cis-*m*-HMC CTCC S₀ EQ, ENERGY= -612.69323065629 , SYMMETRY = C_s, Freq = 14.27075759

C	3.464396355424	0.385910559021	0.042869700178
C	2.287819572766	0.776054171538	0.666613087568
C	1.044087598237	0.267962902874	0.258066500982
C	1.007833758071	-0.646856609591	-0.798158451168
C	2.192552561397	-1.029830664785	-1.414727338559
C	3.417624242693	-0.526016565855	-1.008172917919
O	4.684083307604	0.857508158284	0.412516719229
H	2.330843310117	1.488532353249	1.486931210841
H	0.061711150740	-1.048614692107	-1.126578010597
H	2.157683514192	-1.739701545209	-2.233319310670
H	4.342825430560	-0.822824103011	-1.487077563080
C	-0.119591219356	0.765198043681	1.004042624311
C	-1.447770124776	0.565799912001	0.967641323811
H	0.174821367547	1.471435440449	1.778704437775
H	-2.038467163310	1.115998268096	1.690931690504
C	-2.280425406666	-0.289863215264	0.099753581430
O	-1.942667301421	-1.022935326622	-0.797189220270
O	-3.570745646092	-0.145013688892	0.455777286151
C	-4.505978874686	-0.913817084003	-0.296691917788
H	-4.296610619705	-1.980457138414	-0.196344555218
H	-4.463599816140	-0.644491065792	-1.353695532217
H	-5.482814112011	-0.676268939875	0.118585707916
H	4.580777761777	1.472029252385	1.140328372075

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cis-*m*-HMC CTCC→CCCC TS 3, , ENERGY = -612.690173560067, SYMMETRY = C₁, Freq = -30.69994007

C	2.595627448259	-1.499149841332	0.133781753043
C	1.591419402256	-0.891084263172	0.879979559731
C	0.956196967145	0.250339414591	0.398181314563
C	1.340889527729	0.793535715172	-0.823211196429
C	2.350161827032	0.182301438236	-1.557877354199
C	2.981113147710	-0.958639316953	-1.090015672793
O	3.235779043801	-2.621356168301	0.553448367623
H	1.283453487272	-1.318317282541	1.830191691413
H	0.843419458064	1.678635018452	-1.200855369749
H	2.646087512671	0.599587817748	-2.513791114135
H	3.765151158079	-1.447070342063	-1.655288604990
C	-0.085273101865	0.916970404688	1.220739369946
C	-1.403020243076	0.737202487370	1.150752664331
H	0.282252505961	1.635161137059	1.951792917769
H	-2.064160545312	1.299990301550	1.799227244880
C	-2.068542288360	-0.207855641428	0.220679636766
O	-1.534637323166	-0.972340957061	-0.537643671396
O	-3.404663637307	-0.100225218677	0.343230015917
C	-4.166185620554	-0.961092627260	-0.501287082971
H	-3.935900868472	-2.007417437368	-0.291424207777

H	-3.950820608418	-0.757375675806	-1.551962714375
H	-5.208968742933	-0.747227701340	-0.276928401337
H	2.856527817487	-2.909660541573	1.384754308163

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cis-m-HMC CCCC S₀ EQ, ENERGY = -612.695895463424, SYMMETRY = C₁, Freq = 20.60138893

C	2.379104742982	-1.534512577195	-0.224845181350
C	1.139099941469	-0.925700632572	-0.080488413634
C	1.033537341219	0.468768924658	-0.089796767798
C	2.198835437985	1.231743609359	-0.246484989831
C	3.432189703643	0.613084646488	-0.390252810585
C	3.532625890632	-0.768944532373	-0.380754786806
O	2.520448279246	-2.884390664161	-0.220535188140
H	0.246384029259	-1.525992480967	0.039878781904
H	2.134897683798	2.314184146857	-0.255572091964
H	4.326385984417	1.213581647525	-0.511229046365
H	4.486418647129	-1.270241566387	-0.491525116346
C	-0.219396772962	1.219735583263	0.053837678429
C	-1.518244150095	0.911651268040	0.212185122778
H	-0.043241629254	2.293379372122	0.021904832659
H	-2.207087577434	1.745150044611	0.285750668337
C	-2.205504725114	-0.390304409402	0.305945874164
O	-1.739602883782	-1.504803221545	0.268177214019
O	-3.525508894477	-0.177387660143	0.451605316641
C	-4.332066327876	-1.348077586243	0.556604059234
H	-4.036775967738	-1.942542353992	1.423175065133
H	-4.238221495482	-1.961820011378	-0.341222173388
H	-5.353336135801	-0.991344304113	0.669200845959
H	1.657963797327	-3.288068421543	-0.107976111103

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trans-m-HMC, T₁ m-EQ 1, ENERGY= -612.616232214597, SYMMETRY = C₁, Freq = 40.74361964

C	3.413275475707	0.466986816868	-0.161238067858
C	2.244748985303	0.950326324017	0.396993593093
C	1.072578724439	0.155086058868	0.427390333414
C	1.131777658513	-1.143830261929	-0.131152534588
C	2.310541297725	-1.610288599622	-0.683065931829
C	3.455134196058	-0.821466365131	-0.705428254108
O	4.559597511215	1.193719145679	-0.213195917994
H	2.214483720774	1.952207541969	0.817069138367
H	0.245179953468	-1.767496356672	-0.124463121925
H	2.346400149691	-2.606424449339	-1.109349079313
H	4.382208138066	-1.177198549984	-1.137126444044
C	-0.114064141117	0.661167419424	1.001522870127
C	-1.362995996619	-0.083867667464	1.087589313019
H	-0.106840490232	1.673239183469	1.401780279604
H	-1.587757498414	-0.709986952950	1.947135783964
C	-2.374412544107	0.013868590854	0.044847022567
O	-2.287759804505	0.698446042337	-0.948460326853
O	-3.442161967425	-0.763028811519	0.322928762783
C	-4.486464140917	-0.728633418751	-0.646088859646
H	-4.121776281365	-1.065328087506	-1.618644607850
H	-4.882065741217	0.283642461057	-0.751226802517
H	-5.256249846603	-1.401310452345	-0.274180784011
H	4.405909814530	2.057203119813	0.172868388756

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trans-m-HMC, T₁ m-EQ 2, ENERGY= -612.616800495190, SYMMETRY = C₁, Freq = 35.88231575

C	2.409466190778	0.776410323865	-0.761461966331
C	1.190482782312	0.586330336192	-1.385266031143
C	0.210763651522	-0.265354285753	-0.818246244204
C	0.513131421529	-0.910829972335	0.404084111131
C	1.738613216533	-0.709135263830	1.012052412618
C	2.693355441701	0.127462869045	0.445213509644
O	3.377680863250	1.582975898272	-1.268358935517
H	0.972467489070	1.092651180911	-2.321989250957
H	-0.222608457676	-1.564569316823	0.858350619282
H	1.961842978442	-1.208661922863	1.947989988818
H	3.655182346471	0.292249392472	0.914348814561
C	-1.031925765447	-0.448434595657	-1.465115072583
C	-2.094194501547	-1.311961864952	-0.966723824102
H	-1.218608446104	0.091725089322	-2.391626512451
H	-2.166124353491	-2.352106261805	-1.272422721685
C	-3.142801094220	-0.874643004041	-0.055877341528
O	-4.024356104558	-1.594733375469	0.357698945293
O	-3.020822691169	0.421949627308	0.282767958645
C	-4.005616676955	0.911838152413	1.188736079028
H	-3.973850467883	0.357420459495	2.128714825791
H	-5.005299474011	0.819939168256	0.759395947434
H	-3.756736043101	1.957458153684	1.355578742649
H	3.070745570547	1.970743472292	-2.089136191394

(3) o-HMC

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trans-o-HMC TTTC S₀ EQ, ωB97XD/ 6-311G(d,p),

ENERGY = -612.701190047210, SYMMETRY = C₁, Freq = 21.56701800

C	-3.550730406539	0.533220653888	0.098028769099
C	-2.206929138392	0.898435088776	0.063935618510
C	-1.202752701583	-0.078271546233	-0.048092758076
C	-1.600488285718	-1.415967352631	-0.132470700368
C	-2.934803020451	-1.784841976825	-0.098666764091
C	-3.911940610051	-0.802558380848	0.018551485093
H	-4.313432376426	1.301142014078	0.188977994369
O	-1.816786780024	2.194124758284	0.143513240132
H	-0.841701923437	-2.182026089969	-0.242973379310
H	-3.213164319953	-2.828994212816	-0.170167503715
H	-4.960851142652	-1.074526853861	0.044256165679
C	0.199706576363	0.339428476976	-0.082776367705
C	1.266988991464	-0.452768491024	0.048432649412
H	0.386023963580	1.400064049085	-0.219356281843
H	1.203132492423	-1.520585245851	0.220083974591
C	2.624137351207	0.123304480201	-0.023476028583
O	2.896181423163	1.283687615605	-0.201999345091
O	3.554755091977	-0.834503637893	0.140605797785
C	4.907627237598	-0.388083131048	0.090491248475
H	5.101156270786	0.343061822542	0.877691094936
H	5.126415261015	0.069789988188	-0.876063059632
H	5.517371939363	-1.276896572671	0.237863073936
H	-2.588548893710	2.759416544054	0.193570076394

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trans-o-HMC TTTC S₀ EQ, Spin-flip TD- BHandHLYP/ 6-311G
(*d,p*), ENERGY = -612.552307062700, SYMMETRY = C₁,
Freq = 25.68818619

C	3.533347254946	-0.523418800353	0.040489110369
C	2.193465046469	-0.883652452648	0.023145763314
C	1.193391113375	0.091714354350	-0.019762867376
C	1.590889106328	1.425132683986	-0.048064470900
C	2.921523331318	1.790171791334	-0.030933849057
C	3.894080751514	0.806983770534	0.014228985012
H	4.288922982000	-1.291908466482	0.075175738398
O	1.809420440453	-2.178271148822	0.049896167723
H	0.837915240379	2.191983213707	-0.090639244728
H	3.197136796105	2.829275851779	-0.055206055630
H	4.936606439901	1.074124286511	0.027314441242
C	-0.205324953808	-0.323661625390	-0.036735279338
C	-1.275909752045	0.474863184600	0.021749265754
H	-0.389671429158	-1.382179367072	-0.097134958227
H	-1.216671017685	1.544898008648	0.099202013620
C	-2.623268066553	-0.099764595406	-0.009244613808
O	-2.893409461915	-1.262854990748	-0.097631127110
O	-3.552651825439	0.857773342026	0.077283059468
C	-4.900519606148	0.416627128895	0.060326340429
H	-5.087779835123	-0.270228033979	0.876970192589
H	-5.127314680727	-0.082252874894	-0.874604092799
H	-5.503995562497	1.306319437098	0.168519271932
H	2.571396173984	-2.746081569115	0.069891206957

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trans-o-HMC TTTC ¹ππ* EQ, ENERGY = -612.548597547616,
SYMMETRY = C_s, Freq = 42.09912295

C	2.746260748853	1.052260508707	0.000007060073
C	1.385324973226	1.331070666105	0.000021063456
C	0.369248222906	0.285386901677	0.000017686503
C	0.858735997170	-1.058008323661	-0.000002148828
C	2.216298183242	-1.315261453147	-0.000003852225
C	3.168504539051	-0.276621188212	0.000002850918
H	3.463481798869	1.866970264492	0.000018095168
O	0.911225207755	2.574777254873	0.000033053858
H	0.152992448939	-1.877090390991	0.000001005568
H	2.562831685730	-2.342429171170	-0.000014683198
H	4.225993868053	-0.509081371419	-0.000009172552
C	-0.992478672478	0.637808276384	0.000015658775
C	-2.033581627901	-0.286536560147	0.000002915509
H	-1.266572822406	1.685374704326	0.000026273075
H	-1.870265247754	-1.356786128531	-0.000003879593
C	-3.402053636569	0.177982970196	0.000016296217
O	-3.760368257118	1.342084836959	0.000024561852
O	-4.282181906699	-0.856330024647	0.000008357702
C	-5.652220705221	-0.482132003854	-0.000009905545
H	-5.895836852765	0.108624106513	-0.886517585145
H	-5.895831386371	0.108583456087	0.886529578297
H	-6.215165914002	-1.414103554659	-0.000008450943
H	1.635655542477	3.207236424105	0.000039015063

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o-HMC ¹ππ* *trans* → cis TS 1, ENERGY =
-612.544422090729, SYMMETRY = C₁, Freq = -267.83313398

C	-2.709407147	1.028808345	-0.137196187
C	-1.388046375	1.382551152	-0.343199948
C	-0.349090738	0.385104812	-0.379860500
C	-0.742491544	-0.971877340	-0.155802137
C	-2.060754078	-1.302492386	0.062719510
C	-3.046250063	-0.309102032	0.069622504
H	-3.476255522	1.797106910	-0.112798920
O	-0.990224688	2.651772485	-0.514780002
H	0.031117484	-1.731602168	-0.165222143
H	-2.341424876	-2.337966420	0.214629421
H	-4.084726026	-0.575819813	0.227784087
C	0.982900295	0.746574913	-0.611732490
C	2.052870370	-0.187700379	-0.617745185
H	1.220607485	1.804872667	-0.703478343
H	1.997502223	-1.125192504	-1.165684460
C	3.291873383	0.139581609	0.039100572
O	3.522654008	1.179719648	0.632351232
O	4.213365280	-0.850027785	-0.094290608
C	5.466741007	-0.590396948	0.521818444
H	5.929701654	0.306179814	0.102403011
H	5.349556881	-0.447621761	1.598982385
H	6.083077907	-1.464965052	0.320177550
H	-1.749899965	3.238437008	-0.506242880

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o-HMC *trans*→cis S₀ TS2, ENERGY = -612.618331417662,
SYMMETRY = C₁, Freq = -795.46916356

C	3.424901334206	0.445284485144	-0.150246584648
C	2.269239837744	0.941601798659	0.427818548170
C	1.071697430210	0.169878938585	0.446016001363
C	1.124109046674	-1.113171338086	-0.152476998774
C	2.280729066105	-1.601487047242	-0.725476418061
C	3.437121333182	-0.822852518747	-0.727182874678
H	4.326134008100	1.052018965768	-0.152491622540
O	2.211131700537	2.167709182687	1.003329600339
H	0.221650425550	-1.714824911377	-0.156452176472
H	2.287920248430	-2.586298466151	-1.176934064857
H	4.349237477673	-1.196917500382	-1.176701802389
C	-0.100056357224	0.686975871427	1.031369666294
C	-1.354652612417	-0.047900811817	1.110362058349
H	-0.068297130934	1.690956758466	1.445548515955
H	-1.592553763338	-0.666218628565	1.972997831811
C	-2.356337079890	0.038434381967	0.056873528645
O	-2.251888194070	0.690156620678	-0.956573787944
O	-3.439309935306	-0.714575368343	0.347460006941
C	-4.473459756660	-0.691922149574	-0.631863312214
H	-4.105230297277	-1.060791548163	-1.591436405336
H	-4.853164096623	0.322626040348	-0.769382178306
H	-5.256957236040	-1.342556013131	-0.249240040393
H	3.060221531358	2.602439291856	0.912856427732

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cis-o-HMC S₀ TTCC, ENERGY = -612.694359024300,
SYMMETRY = C₁, Freq = 8.92002368

C	3.430304978546	0.472253897863	-0.045367038479
C	2.269267174114	0.889442079590	0.596677289554
C	1.035496488003	0.248282510760	0.354530924913
C	1.030046857131	-0.822833890160	-0.547384116521
C	2.188203421898	-1.241179819755	-1.184225630500
C	3.389424977642	-0.591586738683	-0.933812936529
H	4.367108363364	0.985299372636	0.152679868829
O	2.287623727570	1.929863224468	1.470703119489
H	0.092153605881	-1.319619728806	-0.747539972440
H	2.150100648304	-2.074000160064	-1.875689139581
H	4.300231330589	-0.909629883378	-1.428497979245
C	-0.124489458858	0.736211344814	1.104024309993
C	-1.454682883256	0.558015065560	1.022422840685
H	0.166601574839	1.411758850493	1.902258035550
H	-2.058617930019	1.091495588425	1.747223202490
C	-2.272480945681	-0.215075372480	0.070018091687
O	-1.917608602072	-0.981742973545	-0.793073078328
O	-3.574171965256	0.051586724053	0.292714311960
C	-4.494434988673	-0.626600002844	-0.557638884225
H	-4.392947675141	-1.708349760421	-0.450980023434
H	-4.323826890512	-0.358815777629	-1.602133178700
H	-5.482738586570	-0.303181143272	-0.238268845583
H	3.186354889037	2.247891717614	1.564041359347

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cis-o-HMC S₀ TTCC → TCCC TS 3, Energy =
-612.689967142678, SYMMETRY = C₁, Freq = -36.22803522

C	2.537984270929	-1.319584899725	0.345222051416
C	1.477014314186	-0.650754270403	0.945652659096
C	1.050186656660	0.582056766370	0.445719151267
C	1.707364367448	1.123311395913	-0.652493996832
C	2.766007485059	0.458444926390	-1.259476865207
C	3.178100809420	-0.766457057006	-0.756031356780
H	2.858979265724	-2.280192312496	0.738091167716
O	0.817100190367	-1.147218704262	2.024427193380
H	1.369626340302	2.076922279999	-1.043320098126
H	3.259387043972	0.893281724775	-2.120107817105
H	4.000773797479	-1.299821549903	-1.218317379472
C	-0.063127215254	1.313015807764	1.100356275864
C	-1.361428613753	1.185559091621	0.836491222417
H	0.224113654100	2.032586667830	1.864732585949
H	-2.087633802491	1.791728741623	1.364832425335
C	-1.918972583555	0.232286670230	-0.152165372340
O	-1.312762135300	-0.581872047799	-0.796645623247
O	-3.252955813926	0.396042025801	-0.240148211758
C	-3.914330111550	-0.470471289164	-1.158620822138
H	-3.532496118586	-0.322669608889	-2.170612705825
H	-3.766769253052	-1.514752203509	-0.876637459005
H	-4.968418360296	-0.206818127666	-1.106464768000
H	1.164467529090	-2.015161096345	2.233528104972

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cis-o-HMC TCCC S₀, ENERGY = -612.691459606038,
SYMMETRY = C₁, Freq = 29.82580145

C	2.329491136287	-1.391103449490	0.213633531578
C	1.234420268629	-0.648392583368	0.647106088397
C	1.133045444262	0.709374514628	0.315859641111
C	2.175307417060	1.294645244986	-0.402998321336
C	3.263898751435	0.556660659499	-0.843772126688
C	3.332740891215	-0.795558703610	-0.536272815120
H	2.395105440785	-2.443908782308	0.472616942171
O	0.268258221265	-1.191871434404	1.424396777966
H	2.110513373988	2.351990519460	-0.639031294243
H	4.049035548667	1.031916324490	-1.418787176295
H	4.174849300656	-1.391073123818	-0.869843170119
C	0.001661035541	1.553912500482	0.743357329196
C	-1.308268865665	1.347435097627	0.593605289675
H	0.291079691929	2.483162562555	1.230396290175
H	-2.007946581046	2.071809049347	0.993520260537
C	-1.927233884642	0.216179977196	-0.132199583347
O	-1.379294707479	-0.581192296087	-0.846766217889
O	-3.257502833417	0.212105947654	0.084926298694
C	-3.981411167254	-0.815192817124	-0.585589312515
H	-3.856128452981	-0.732680790379	-1.666990332363
H	-3.636233767814	-1.800740637004	-0.266712971000
H	-5.023886321814	-0.670320457551	-0.310337107741
H	0.367469127237	-2.144475844939	1.428451323605

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cis-o-HMC S₀ TCCC → CCCC TS 4, Energy =
-612.691113783997, Symmetry = C₁, Freq = -236.77249749

C	2.421565790639	0.706630719799	-0.945511261609
C	1.348217348739	0.706324269345	-0.058807418515
C	1.100000533356	-0.414424672390	0.741005532047
C	1.990756312611	-1.488770600432	0.674642976882
C	3.055399430164	-1.494672041185	-0.212455572765
C	3.262274336781	-0.392208762550	-1.033172978725
H	2.601163610452	1.587046302848	-1.553963168020
O	0.560385983101	1.804152013283	0.093070075479
H	1.817359104400	-2.348096135450	1.314577199347
H	3.718501464175	-2.349745351581	-0.262485775390
H	4.091141375073	-0.378449336013	-1.731698919166
C	-0.037198973450	-0.500415643319	1.674409246125
C	-1.334880110782	-0.265554500947	1.462010487301
H	0.227274776867	-0.843741881794	2.672867321831
H	-2.030957996592	-0.387255445920	2.283383850779
C	-1.963787663754	0.093026332517	0.173054707083
O	-1.442730412582	0.163435632476	-0.910878657210
O	-3.279878358830	0.311663660019	0.361888157557
C	-4.021717552346	0.636931216821	-0.809824413477
H	-3.949662895196	-0.164888428778	-1.547133215032
H	-3.649798612804	1.560739449682	-1.257657224849
H	-5.051336097965	0.762475199959	-0.481985886484
H	0.364826719273	2.165283126642	-0.772652542701

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cis *o*-HMC CCCC S₀, ENERGY = -612.700180292624SYMMETRY = C₁ Freq = 31.18604157

C	2.585293297088	-1.302810441159	0.004430088525
C	1.346008574401	-0.757114169211	-0.349917264806
C	1.135831563565	0.630197789954	-0.203802252789
C	2.197539525714	1.407294601477	0.296671941452
C	3.403129684890	0.855151095945	0.675940172391
C	3.597811544270	-0.516183471292	0.514779542379
H	2.712782997050	-2.369484419110	-0.133957438240
O	0.447107786935	-1.596735335640	-0.885851349347
H	2.051886846339	2.479457561536	0.385145050954
H	4.191606849040	1.483371835753	1.071852544173
H	4.544471767111	-0.969087023526	0.787524595166
C	-0.035169926499	1.390336294851	-0.661493553889
C	-1.367710075786	1.217555460136	-0.642021310407
H	0.258919163014	2.351130428547	-1.080815655598
H	-1.982551467358	2.012592593047	-1.046319364667
C	-2.139648708820	0.143575000302	-0.011052345637
O	-1.723774718240	-0.925209952120	0.396431874314
O	-3.423236573577	0.486088715024	0.099253799146
C	-4.278375072666	-0.476897178454	0.719605157139
H	-3.958361002968	-0.666643004444	1.745163463308
H	-4.264511792427	-1.414648502255	0.162270597183
H	-5.271800602985	-0.035580518504	0.703861225124
H	-0.427626220538	-1.412430885706	-0.488223875389

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trans-*o*-HMC, ¹ππ*/¹ππ*, MECI 2, ENERGY =-612.539537303395, SYMMETRY = C₁

C	-3.561388706218	-0.509936752771	-0.002345679335
C	-2.226062739502	-0.888397108995	-0.001808499743
C	-1.173473552378	0.076528735585	0.001126441319
C	-1.567080467638	1.433290342987	0.004337641664
C	-2.900057972616	1.805688341764	0.003652157060
C	-3.905561088489	0.838030882657	0.000232681435
H	-4.334022665810	-1.273711834894	-0.004718467936
O	-1.851565170609	-2.187062046260	-0.004391414109
H	-0.804703875219	2.202516135651	0.008123299431
H	-3.163833510001	2.856919630311	0.006041726338
H	-4.949040098809	1.128907706058	-0.000128718211
C	0.183290840646	-0.365532889675	0.000477568943
C	1.291982301510	0.478112356749	-0.003181274267
H	0.350983524781	-1.434022336710	0.002281897955
H	1.216594521239	1.558876970813	-0.008708459362
C	2.595241845833	-0.018020762828	0.000259677142
O	2.889554672655	-1.259031992169	0.011931785476
O	3.610464900970	0.863176834396	-0.009091216239
C	4.939623125470	0.342043010555	-0.000726981125
H	5.124643055566	-0.271455675664	-0.885192138521
H	5.121561169180	-0.250088950420	0.898792895781
H	5.588073537755	1.214958519529	-0.009863580108
H	-2.631930926980	-2.744418851229	-0.006111665083

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trans-*o*-HMC ¹ππ*EQ3, ENERGY = -612.541833299822,SYMMETRY = C₁, Freq = 17.79112347

C	3.553524303194	0.516092654725	0.031189195311
C	2.217275703213	0.889461705162	0.026803107813
C	1.185798430910	-0.077341114615	-0.020183506940
C	1.584970161995	-1.424097246575	-0.070067416605
C	2.918769316098	-1.798292651850	-0.062281826433
C	3.910895313061	-0.826828799322	-0.011264990363
H	4.322293096927	1.283335485644	0.070122454579
O	1.839412172802	2.196845129116	0.070204667408
H	0.826281469602	-2.196146412087	-0.124515759747
H	3.184577470135	-2.848131461311	-0.101593778286
H	4.957838586896	-1.105994326228	-0.007724622220
C	-0.186888180103	0.353615090815	-0.014993210848
C	-1.291206159888	-0.490965193174	0.037450993881
H	-0.346250591635	1.423033994466	-0.043722011090
H	-1.212912887605	-1.568234485717	0.121690303547
C	-2.581163506392	-0.020994010983	-0.013095785075
O	-2.889567525454	1.240195861736	-0.176147158961
O	-3.632199344062	-0.837754822184	0.112964592102
C	-4.948912450453	-0.317440263392	-0.101424902121
H	-5.051776000078	0.076550935419	-1.114597116085
H	-5.186177327662	0.459463447429	0.628017130630
H	-5.612407702308	-1.167143791502	0.035323720575
H	2.622206848800	2.748054689426	0.092839777953

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trans-*o*-HMC ¹ππ*/³ππ* (S₁/T₃) MESX1, SYMMETRY = C_s,

ENERGY = -612.548495729152

C	3.578909193468	0.523180865276	-0.000026683778
C	2.233595275568	0.890911253967	0.000049363836
C	1.154555459830	-0.085846038784	-0.000042580200
C	1.552122146132	-1.453564206227	0.000034007236
C	2.894816429145	-1.803613697520	-0.000025723177
C	3.914960523741	-0.829334894793	0.000026146282
H	4.346641035816	1.290484119014	0.000003260573
O	1.846213787998	2.165825138293	-0.000002965553
H	0.794685265167	-2.225210058916	0.000004094549
H	3.170717535159	-2.851799608059	0.000008317344
H	4.954860231199	-1.130492297151	-0.000003411207
C	-0.187038760985	0.361737340589	-0.000003278658
C	-1.291316652484	-0.480218332357	0.000078203227
H	-0.383274832435	1.426650926359	0.000000699545
H	-1.209870936196	-1.559853221624	-0.000011545080
C	-2.622172935372	0.086841511351	-0.000183977708
O	-2.890897947786	1.274295937216	0.000058803617
O	-3.577648432998	-0.877163375194	0.000067742565
C	-4.915605570031	-0.399835816142	-0.000027406580
H	-5.113357731695	0.207696022282	-0.886527874761
H	-5.113338506969	0.20764415927	0.886497101600
H	-5.547660801140	-1.286292529965	-0.000005492657
H	2.612658058086	2.746288726314	0.000006667825

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trans-o-HMC $^1\pi\pi^*/^3\pi\pi^*$ (S_1/T_d) MESX2, ENERGY =
-612.545970949338, SYMMETRY = C_s

C	3.571336411622	0.513380752716	0.000063011793
C	2.235109386475	0.892630642954	-0.000103600019
C	1.164895810056	-0.071928415508	0.000112526603
C	1.555784550324	-1.436204270295	-0.000059635577
C	2.889599701673	-1.803428336515	0.000056214857
C	3.905558002984	-0.838075947315	-0.000044534848
H	4.345341852083	1.275129331069	-0.000008074316
O	1.859759229624	2.181186071221	0.000023155732
H	0.792622869567	-2.203534616743	0.000013680856
H	3.154286929999	-2.854519652864	-0.000000967054
H	4.946063350404	-1.138456320217	0.000002309796
C	-0.181112382449	0.378220747515	-0.000046812066
C	-1.286918273831	-0.463517885875	0.000036964703
H	-0.359221816207	1.445407397669	0.000018081130
H	-1.206347297884	-1.544029889459	-0.000004628876
C	-2.610134675758	0.048357849578	-0.000056891891
O	-2.902153403953	1.261574481630	0.000026934606
O	-3.585792138877	-0.889332977957	0.000008759530
C	-4.923652172314	-0.404982945809	-0.000010865982
H	-5.121961552721	0.197883570754	-0.889574778685
H	-5.121976707098	0.197887222901	0.889546577210
H	-5.554509842353	-1.291670755372	-0.000021927612
H	2.635974001980	2.746386125896	-0.000002031053

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trans-o-HMC S/S_0 MECI 1, Spin-Flip TD-BHandHLYP/6-311G
(d,p), ENERGY = -612.430337468512 SYMMETRY = C_1

C	-3.296653014	0.161380230	0.450802508
C	-2.154778616	0.837197827	0.058969762
C	-1.010632090	0.103127910	-0.376795565
C	-1.084315601	-1.313796656	-0.400343263
C	-2.218492012	-1.966217995	-0.016928073
C	-3.318332631	-1.218477340	0.411713659
H	-4.160394128	0.710249005	0.786258715
O	-2.081283154	2.160474256	0.065598275
H	-0.198905165	-1.824823677	-0.725229269
H	-2.270569818	-3.039103447	-0.031584859
H	-4.214120505	-1.728409889	0.722697517
C	0.167790370	0.751351074	-0.716568127
C	1.386062260	0.119392233	-1.130856876
H	0.101765035	1.833000005	-0.624323825
H	1.699001424	0.192712419	-2.154918327
C	2.283945272	0.084467661	-0.078901851
O	1.980131899	0.340978196	1.092014614
O	3.558667417	-0.270151508	-0.399512786
C	4.454960024	-0.333380896	0.684019850
H	4.591664226	0.639847839	1.144860370
H	4.106418491	-1.020120668	1.447945440
H	5.394849781	-0.681574789	0.274421257
H	-2.883979575	2.546783131	0.403054360

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trans-o-HMC S/S_0 MECI 2, Spin-Flip TD-BHandHLYP/6-311G
(d,p), ENERGY = -612.430554404446, SYMMETRY = C_1

C	3.317798146780	0.304348576792	-0.358065109936
C	2.103044318918	0.867077246531	-0.003440040341
C	0.998705033411	0.022814061651	0.337351141235
C	1.158937565994	-1.385420425107	0.194538781586
C	2.352903181358	-1.919790866472	-0.175594576089
C	3.433062749484	-1.064489235941	-0.439050830127
H	4.138171968760	0.955338935819	-0.597539518619
O	2.026826125286	2.188397263632	-0.013888454523
H	0.300345308325	-1.987790380033	0.420332425399
H	2.476440680811	-2.983315596069	-0.265506164294
H	4.379442980327	-1.486907524068	-0.730718154100
C	-0.172805410036	0.540226989235	0.858567269619
C	-1.386492980262	-0.172450421034	1.124209634582
H	-0.140190935060	1.611267431056	1.076227899880
H	-1.671037521445	-0.442303580112	2.122273788339
C	-2.302359535886	0.044964307737	0.104177179732
O	-2.026788942093	0.643736842395	-0.940032502689
O	-3.549628906610	-0.442544670508	0.319224258552
C	-4.472865571528	-0.223529235816	-0.722623079501
H	-4.121556138715	-0.647657609775	-1.656843624711
H	-4.652452306976	0.835500561951	-0.877146018981
H	-5.388771255779	-0.711300293192	-0.414871011815
H	1.123718732751	2.489404909133	0.041767293118

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trans-o-HMC S/S_0 MECI 3, Spin-Flip TD-BHandHLYP/6-311G
(d,p), ENERGY = -612.429560072449 SYMMETRY = C_1

C	3.149254038231	0.361288882804	0.411854269031
C	1.970216617093	0.882340856791	-0.091929405552
C	0.892038102758	0.007837760571	-0.419017609513
C	1.060876992079	-1.384285395172	-0.207939031079
C	2.227163063076	-1.884183181850	0.291929110659
C	3.266231065820	-1.001790367962	0.598193434434
H	3.967204806386	1.017226793168	0.657844378050
O	1.803717674951	2.182680883615	-0.292309809517
H	0.220385794320	-2.000938190912	-0.461128758173
H	2.352070636757	-2.938927790547	0.453279246608
H	4.189326962388	-1.390179685276	0.993465846713
C	-0.308777940746	0.503112407221	-0.918271975371
C	-1.438238800083	-0.277606270952	-1.298299438015
H	-0.307568783476	1.587763072104	-1.013533109916
H	-1.637211112125	-0.377806641012	-2.349799532018
C	-2.527621241583	-0.226527802237	-0.432400785449
O	-3.675496446586	-0.587605034615	-0.556496774893
O	-2.110667174136	0.341065178062	0.783275955400
C	-3.095295759347	0.440465026043	1.783158765587
H	-2.622913472656	0.927520881830	2.628102327488
H	-3.456140649616	-0.538950295854	2.080702137129
H	-3.944477518114	1.025869819854	1.447385367247
H	2.577580661704	2.672314674903	-0.029968925966

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trans-o-HMC S/S₀ MECI 4, Spin-Flip TD-BHandHLYP/6-311G
(*d,p*), ENERGY = -612.423962050049, SYMMETRY = C₁

C	3.310500733075	0.081034176120	0.176199435457
C	2.160075529129	0.793025524556	-0.110065165921
C	0.930606602336	0.104843133839	-0.321655719914
C	0.928992218365	-1.308491903337	-0.226450010094
C	2.071407456383	-2.000446118820	0.055501078333
C	3.259430874609	-1.296784175248	0.258326643130
H	4.239498668611	0.601878816063	0.337381766223
O	2.153712587266	2.119367355322	-0.206634929242
H	-0.013617077599	-1.798147050187	-0.377297432126
H	2.060365419630	-3.072070147817	0.132417091601
H	4.162781223390	-1.835963704238	0.486545193825
C	-0.245254029314	0.807683456161	-0.561086320769
C	-1.545414594828	0.231272621593	-0.770333191072
H	-0.118570097220	1.884947113042	-0.571467639655
H	-1.938106713427	0.147424437567	-1.764157621051
C	-2.276074725168	0.205116553596	0.413985162088
O	-1.779655896676	0.520452049676	1.493529558401
O	-3.578589287095	-0.186865657152	0.424784745620
C	-4.182499679308	-0.579874524562	-0.774957863280
H	-4.227550894129	0.239655776500	-1.490174112057
H	-5.191097456619	-0.884769453103	-0.528427593354
H	-3.657788334068	-1.417329083399	-1.230730034111
H	3.012148870636	2.479641003666	-0.006600591336

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trans-o-HMC S/S₀ MECI 5, Spin-Flip TD-BHandHLYP/6-311G
(*d,p*), ENERGY = -612.419839088550, SYMMETRY = C₁

C	2.621221042319	-1.240920720173	-0.356056680135
C	1.369723681851	-0.905107927935	0.150913781676
C	1.063938667552	0.466005202108	0.396859203588
C	2.066648588743	1.426029784680	0.096540565999
C	3.286218681788	1.081712113512	-0.402051020576
C	3.556009572652	-0.270164152783	-0.629597154444
H	2.849149323671	-2.277654424196	-0.540583258225
O	0.475223678706	-1.836013590247	0.415122764822
H	1.827075194213	2.459788501492	0.273318000707
H	4.025675475602	1.829095604746	-0.623039398896
H	4.512268328311	-0.563551204758	-1.026953970271
C	-0.152855058168	0.946349940861	0.889057247107
C	-1.348449102117	0.243429799009	1.263472370203
H	-0.120115518699	2.028769297827	1.011072237151
H	-1.589219670566	-0.059141458736	2.260357803490
C	-2.136462954494	0.246055451269	0.151820435231
O	-1.707536214253	0.772133267340	-0.903992978698
O	-3.370756591410	-0.303211737216	0.199275663800
C	-4.131419251628	-0.189515983420	-0.981538490697
H	-5.077341120398	-0.672585635701	-0.772500345188
H	-4.298569468869	0.849222392035	-1.247142932555
H	-3.642834207432	-0.679107405177	-1.817069314390
H	0.810229253234	-2.696505415541	0.179559094194

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trans-o-HMC S/S₀ MECI 6, Spin-Flip TD-BHandHLYP/6-311G
(*d,p*), ENERGY = -612.405477125300, SYMMETRY = C₁

C	3.531473582916	0.472882233906	0.137388749935
C	2.240101371093	0.894355535237	-0.008509561586
C	1.172294856538	-0.069437455969	-0.113702679350
C	1.523877217752	-1.439593222474	-0.075447697066
C	2.823436204827	-1.848882359455	0.109461469166
C	3.823858882460	-0.895793595913	0.195235982127
H	4.327769179627	1.195795327031	0.212127831548
O	1.892470396711	2.192616100715	-0.049663804624
H	-1.353343761929	-0.919847136243	-1.405359905858
H	3.080444906939	-2.894326083596	0.161136667670
H	4.852565663688	-1.202337149056	0.299315001995
C	-0.128397791592	0.358151004524	-0.236870026686
C	-1.280912896218	-0.562087653316	-0.375595236572
H	-0.341257718356	1.412103696076	-0.236393004532
H	-1.150443770848	-1.461732149690	0.214872634452
C	-2.597536761609	0.083541775253	-0.040719384612
O	-2.772175438395	1.243605007457	0.172282217635
O	-3.572583350968	-0.819680721672	-0.027265237711
C	-4.876998711070	-0.330367345377	0.257334799638
H	-4.905626212455	0.122841768998	1.240689527211
H	-5.175637677484	0.405436998891	-0.479269309558
H	-5.528299698015	-1.191009860421	0.218861603321
H	2.661094094406	2.742518667818	0.063669550981

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trans-o-HMC S/S₀ MECI 7, Spin-Flip TD-BHandHLYP/6-311G
(*d,p*), ENERGY = -612.397390974317, SYMMETRY = C₁

C	3.530280454093	0.502381992102	0.003707479628
C	2.202879700447	0.880451442078	-0.001013955596
C	1.170614340252	-0.079051786614	-0.003850679630
C	1.561580478852	-1.425121765971	-0.003244273651
C	2.886855689460	-1.803224476105	0.001225824213
C	3.879179160335	-0.837856580115	0.005084844049
H	4.296385182228	1.261980354839	0.006489947961
O	1.836137506744	2.184678240925	-0.001726899986
H	0.803289878212	-2.187750883000	-0.006048225595
H	3.146619285851	-2.847400267879	0.001594531602
H	4.917475875905	-1.119734243403	0.009145064319
C	-0.191530042541	0.356740076439	-0.005116120527
C	-1.305874153217	-0.470855844453	-0.004396637221
H	-0.357703539312	1.417624717658	-0.005416032662
H	-1.222705999218	-1.541937381973	-0.005699827361
C	-2.581815988018	0.002822981151	-0.000146830544
O	-2.886688621154	1.286343771645	0.003669456173
O	-3.610099541498	-0.871621251244	0.001675826323
C	-4.898282168404	-0.426267727775	0.001841441850
H	-3.850955239302	1.358958818329	0.005818639876
H	-5.419006146625	-0.519715666928	0.938049697106
H	-5.419832736686	-0.519820183395	-0.933862516301
H	2.610374771665	2.735734948248	0.002858713308

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trans-o-HMC S/S₀ MECI 8, Spin-Flip TD-BHandHLYP/6-311G
(*d,p*), ENERGY = -612.388870150583, SYMMETRY = C₁

C	2.859833255157	1.249719602950	-0.006442560109
C	1.573150236674	0.796291935675	0.007229748755
C	1.259028172938	-0.595203166601	0.003444978665
C	2.376575406653	-1.480474755979	-0.018053254816
C	3.663567028403	-1.005911908264	-0.031940777450
C	3.930869297169	0.356637965504	-0.025991276297
H	3.042189934956	2.313733734551	-0.003388302903
O	0.494911222299	1.652124956906	0.023706822507
H	2.187646098624	-2.538689670569	-0.021851336198
H	4.477805693110	-1.710295750328	-0.047805904086
H	4.940235733110	0.724503460902	-0.035491017704
C	-0.033377749263	-1.008300138527	0.021070081295
C	-1.376004935536	-1.224981499519	0.018208670013
H	-1.227057726253	1.250266117005	0.026457377710
H	-1.723449752599	-2.249135529346	0.005546667062
C	-2.359941501558	-0.275609731386	0.037904878886
O	-2.168398828270	1.035277398378	0.045209298211
O	-3.632342139886	-0.658791805315	0.073697639295
C	-4.635649289210	0.316894490494	-0.142810852725
H	-4.519935972813	0.784529526998	-1.114844711768
H	-4.612558661754	1.079432584968	0.626439426382
H	-5.571671214014	-0.221033814821	-0.102130740880
H	0.793807288016	2.554925255602	0.039449134781

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trans-o-HMC S/S₀ MECI 9, Spin-Flip TD-BHandHLYP/6-311G
(*d,p*), ENERGY = -612.382248077824, SYMMETRY = C₁

C	3.027267666011	0.441236140467	1.139197518894
C	2.244461592742	0.937696694802	-0.004314259256
C	1.111464901239	0.116739593144	-0.357507682674
C	1.581532349135	-1.203955833538	-0.707902246490
C	2.696230287779	-1.649946104723	-0.079852192395
C	3.336593175749	-0.856488196211	0.963246302925
H	3.390925458077	1.042010596938	1.955375962184
O	2.929340982867	1.416995015556	-1.041784517674
H	0.986722645277	-1.873045276566	-1.309238917448
H	3.049226079477	-2.652412734898	-0.247656797263
H	4.024231734476	-1.349897401934	1.632413767217
C	-0.224532758442	0.438669985899	-0.046631298169
C	-1.311893029749	-0.337868972164	-0.246225972021
H	-0.406120548858	1.421436000591	0.358855517749
H	-1.255732711170	-1.335511467979	-0.641063161464
C	-2.638794879055	0.176210505750	0.074675004423
O	-2.885884776842	1.261565102374	0.521830301448
O	-3.587517504384	-0.730748221353	-0.188767221137
C	-4.918814125979	-0.331346047079	0.089739604077
H	-5.196218287542	0.523832503825	-0.515622050547
H	-5.028964947446	-0.067980712262	1.134990789240
H	-5.540065689179	-1.181442812965	-0.153270705980
H	3.837505744389	1.577039234775	-0.783145496143

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trans-o-HMC S/S₀ MECI 10, Spin-Flip TD-BHandHLYP/6-311G
(*d,p*), ENERGY = -612.380755355549, SYMMETRY = C₁

C	2.870893537311	0.755445253367	1.095084059278
C	2.061433970467	1.005220087006	-0.108842575585
C	1.048596868535	0.012145968936	-0.371310783933
C	1.688681989288	-1.267925440903	-0.551097896224
C	2.840232470135	-1.488375241536	0.130917858373
C	3.352024742593	-0.501849979740	1.074071355555
H	3.128794524345	1.488257656990	1.840449581200
O	2.708221749460	1.437987533613	-1.189819944157
H	1.193661864014	-2.077937018253	-1.062810151515
H	3.318496378179	-2.451303707745	0.090196338308
H	4.084082325877	-0.819960921537	1.800039368622
C	-0.329949359970	0.200373828766	-0.132377333046
C	-1.296069632218	-0.735850358783	-0.252628460126
H	-0.635907642891	1.198801817886	0.131481390333
H	-1.079309974304	-1.757796528915	-0.504938810478
C	-2.715737501297	-0.464531736811	-0.064613343361
O	-3.574493505016	-1.294529421045	-0.169762078095
O	-2.982299016040	0.812537836975	0.242857833873
C	-4.350496394983	1.128958780313	0.433831687299
H	-4.383010398715	2.190387582692	0.634933622852
H	-4.758940709462	0.574715385165	1.270791518819
H	-4.925749577437	0.894697468841	-0.453843059887
H	3.583825349025	1.738078335498	-0.942744480578

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trans-o-HMC T₁ o-EQ 1, ENERGY = -612.617603345583,
Symmetry = C₁, Freq = 38.90162402

C	0.358005199396	0.530659092026	0.427979462477
C	1.394981777557	1.426232554305	0.623301639011
C	2.751450032609	1.020893887733	0.459636486840
C	2.979706380821	-0.329093150180	0.094101176450
C	1.940027686481	-1.215442565763	-0.100046669760
C	0.623289856021	-0.788767956656	0.066880114962
H	-0.668270002496	0.862373751935	0.558640192242
O	1.185398801550	2.719355914970	0.972041946369
H	4.005170778844	-0.660771758319	-0.028573937057
H	2.147689836892	-2.241988223167	-0.377199142844
H	-0.199310964384	-1.478193950233	-0.081253059316
C	3.798161065261	1.937239479154	0.666006856129
C	5.206346823007	1.606223706806	0.497149948615
H	3.546965654762	2.948355691400	0.972227320982
H	5.708479396939	1.755758859930	-0.455287575973
C	6.006923692399	1.098920802901	1.601420430282
O	5.602327831352	0.892753689605	2.722527222064
O	7.283441422745	0.876056196506	1.219798312125
C	8.141984532228	0.374974834665	2.239961555152
H	7.775473068409	-0.581551318558	2.618369621179
H	8.205411617921	1.079254990556	3.072045639361
H	9.116135493959	0.250947535130	1.771702688980
H	0.245307295721	2.872682177251	1.076315240743

trans-o-HMC T₁ o-EQ 2, ENERGY = -612.618240997089,

Symmetry = C₁, Freq = 32.68766507

C	2.413656231231	0.773212923394	-0.743048136188
C	1.200035801888	0.590035837731	-1.382697147996
C	0.200946396777	-0.259155761871	-0.825125147901
C	0.508808191972	-0.894170675773	0.403609669145
C	1.722092984184	-0.707449227311	1.034398273080
C	2.680453994287	0.128434125488	0.463166685411
H	3.160725130805	1.424948263594	-1.187499119395
O	0.896766133363	1.195186507146	-2.557649129981
H	-0.239434436760	-1.542093515896	0.847638830106
H	1.927303428301	-1.207861345799	1.973140292921
H	3.635277199467	0.281981722110	0.951680170478
C	-1.032523508775	-0.434426109525	-1.479236036742
C	-2.093751796278	-1.299600876531	-0.982098747393
H	-1.208576148087	0.107089346670	-2.404039787270
H	-2.170437035136	-2.336093192298	-1.299238552260
C	-3.138768731906	-0.871817985663	-0.063967741701
O	-4.024634662689	-1.593416129187	0.339297463942
O	-3.009663208900	0.418280252531	0.298161628944
C	-3.994341796523	0.897786842660	1.208747600355
H	-3.968427927903	0.328595169605	2.140187179690
H	-4.993439371262	0.817465551338	0.775606382466
H	-3.741517313672	1.939620727393	1.392843569966
H	1.633401791615	1.742613343204	-2.833095340678