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Supporting Information

An Exploration of the Solvent- and Acid-catalyzed Mutarotation Mechanisms of Lactose in Aqueous Solution

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Table S1 Changes of Gibbs free energies (ΔG-s) and electronic energies (ΔE-s) for the solvent-catalyzed mutarotation processes of α-lactose in aqueous solution.

	B3LYP-D3		B3PW91-D3		PBE1PBE-D3	
	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE
Direct reaction mechanism						
RC⟶TS1	42.5	43.0	42.5	43.0	43.7	44.2
RC⟶IM1	7.3	8.5	10.4	11.6	12.1	13.3
IM1⟶TS_R	2.6	2.3	2.3	2.0	2.0	1.7
IM1⟶IM2	-0.4	-0.2	-0.4	-0.2	-0.6	-0.3
IM2⟶TS2	34.3	33.3	31.1	30.1	30.6	29.5
IM2⟶PC	-3.9	-5.5	-7.0	-8.7	-8.3	-10.0
One-water-mediated reaction mechanism						
RC_w⟶$TS1_w$	25.4	24.5	24.4	23.5	25.8	25.0
RC_w⟶$IM1_w$	6.6	7.8	9.6	10.9	11.2	12.5
$IM1_w$⟶$IM2_w$	0.5	0.6	0.6	0.6	0.5	0.6
$IM2_w$⟶$TS2_w$	18.1	15.7	14.2	11.8	13.9	11.5
$IM2_w$⟶PC_w	-7.3	-7.4	-10.6	-10.7	-12.2	-12.3
Two-water-mediated reaction mechanism						
RC_{2w}⟶$TS1_{2w}$	22.1	20.4	20.9	19.1	22.1	20.4
RC_{2w}⟶$IM1_{2w}$	5.9	7.0	9.6	10.1	10.4	11.5
$IM1_{2w}$⟶$IM2_{2w}$	0.3	0.1	0.4	0.2	0.3	0.1
$IM2_{2w}$⟶$TS2_{2w}$	18.8	13.4	14.7	9.2	14.4	8.9
$IM2_{2w}$⟶PC_{2w}	-5.6	-6.4	-8.6	-9.4	-10.1	-10.9
Three-water-mediated reaction mechanism						

$RC_{3w} \rightarrow TS1_{3w}$	21.8	21.1	20.2	19.5	21.2	20.5
$RC_{3w} \rightarrow IM1_{3w}$	6.8	8.6	9.7	11.5	11.3	13.1
$IM1_{3w} \rightarrow IM2_{3w}$	-0.4	-0.1	-0.3	0.0	-0.4	-0.1
$IM2_{3w} \rightarrow TS2_{3w}$	18.5	14.9	14.3	10.7	13.7	10.1
$IM2_{3w} \rightarrow PC_{3w}$	-4.2	-6.4	-7.0	-9.2	-8.6	-10.8

Table S2 Changes of Gibbs free energies (ΔG-s) and electronic energies (ΔE-s) for the HAc-catalyzed mutarotation processes of α-lactose in aqueous solution.

	B3LYP-D3		B3PW91-D3		PBE1PBE-D3	
	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE
Direct reaction mechanism						
$RC_{HAc} \rightarrow TS1_{HAc}$	13.5	12.8	13.7	13.0	15.0	14.3
$RC_{HAc} \rightarrow IM1_{HAc}$	6.9	7.7	9.9	10.7	11.4	12.2
$IM1_{HA}{}^{c} \rightarrow IM2_{HAc}$	2.1	2.2	2.3	2.4	2.1	2.2
$IM2_{HA}{}^{c} \rightarrow TS2_{HAc}$	5.0	3.3	2.2	0.5	2.2	0.5
$IM2_{HAc} \rightarrow PC_{HAc}$	-8.2	-9.1	-11.3	-12.1	-12.7	-13.6
One-water-mediated reaction mechanism						

$RC_{HAc+w} \rightarrow TS1_{HAc+w}$	17.2	16.9	17.4	17.0	19.2	18.9
$RC_{HAc+w} \rightarrow IM1_{HAc+w}$	6.9	7.9	9.6	10.7	11.1	12.2
$IM1_{HAc+w} \rightarrow IM2_{HAc+w}$	0.0	0.0	0.1	0.1	0.0	0.0
$IM2_{HAc+w} \rightarrow TS2_{HAc+w}$	9.2	9.2	6.9	6.9	7.3	7.4
$IM2_{HAc+w} \rightarrow PC_{HAc+w}$	-5.7	-7.7	-8.5	-10.5	-10.0	-11.9

Table S3 Changes of Gibbs free energies (ΔG-s) and electronic energies (ΔE-s) for the TFA-catalyzed mutarotation processes of α-lactose in aqueous solution.

	B3LYP-D3		B3PW91-D3		PBE1PBE-D3	
	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE
Direct reaction mechanism						
$RC_{TFA} \rightarrow TS1_{TFA}$	8.7	8.7	10.3	10.2	11.9	11.9
$RC_{TFA} \rightarrow IM1_{TFA}$	6.8	7.3	9.7	10.3	11.2	11.7
$IM1_{TFA} \rightarrow IM2_{TFA}$	-0.4	0.1	-0.3	0.2	-0.4	0.1
$IM2_{TFA} \rightarrow TS2_{TFA}$	2.5	1.3	1.2	0.0	1.5	0.2
$IM2_{TFA} \rightarrow PC_{TFA}$	-5.7	-6.3	-8.4	-9.1	-9.9	-10.5
One-water-mediated reaction mechanism						
$RC_{TFA+w} \rightarrow TS1_{TFA+w}$	10.8	9.9	12.0	11.1	13.8	12.9
$RC_{TFA+w} \rightarrow IM1_{TFA+w}$	6.6	6.3	9.6	9.3	10.7	10.4
$IM1_{TFA+w} \rightarrow IM2_{TFA+w}$	0.1	0.3	-0.1	0.0	0.1	0.2
$IM2_{TFA+w} \rightarrow TS2_{TFA+w}$	2.8	3.0	1.5	1.6	1.9	2.1
$IM2_{TFA+w} \rightarrow PC_{TFA+w}$	-6.0	-5.7	-8.6	-8.3	-10.0	-9.7

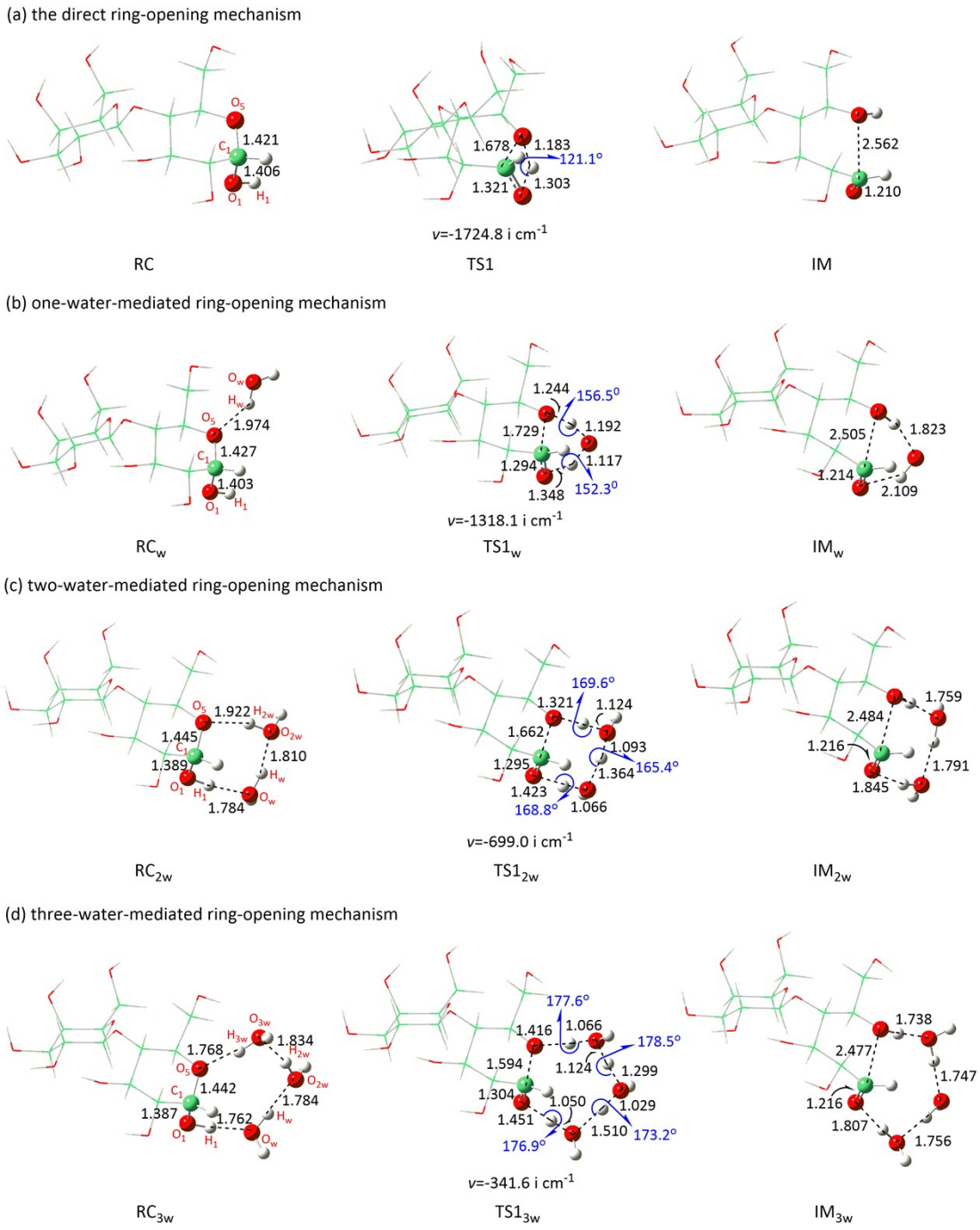

Fig. S1 B3LYP-D3/6-311++G(d,p) optimized structures (Å) of all the stationary points in the solvent-catalyzed ring-opening step of α-lactose (*v* represents for the single imaginary frequency of the transition state).

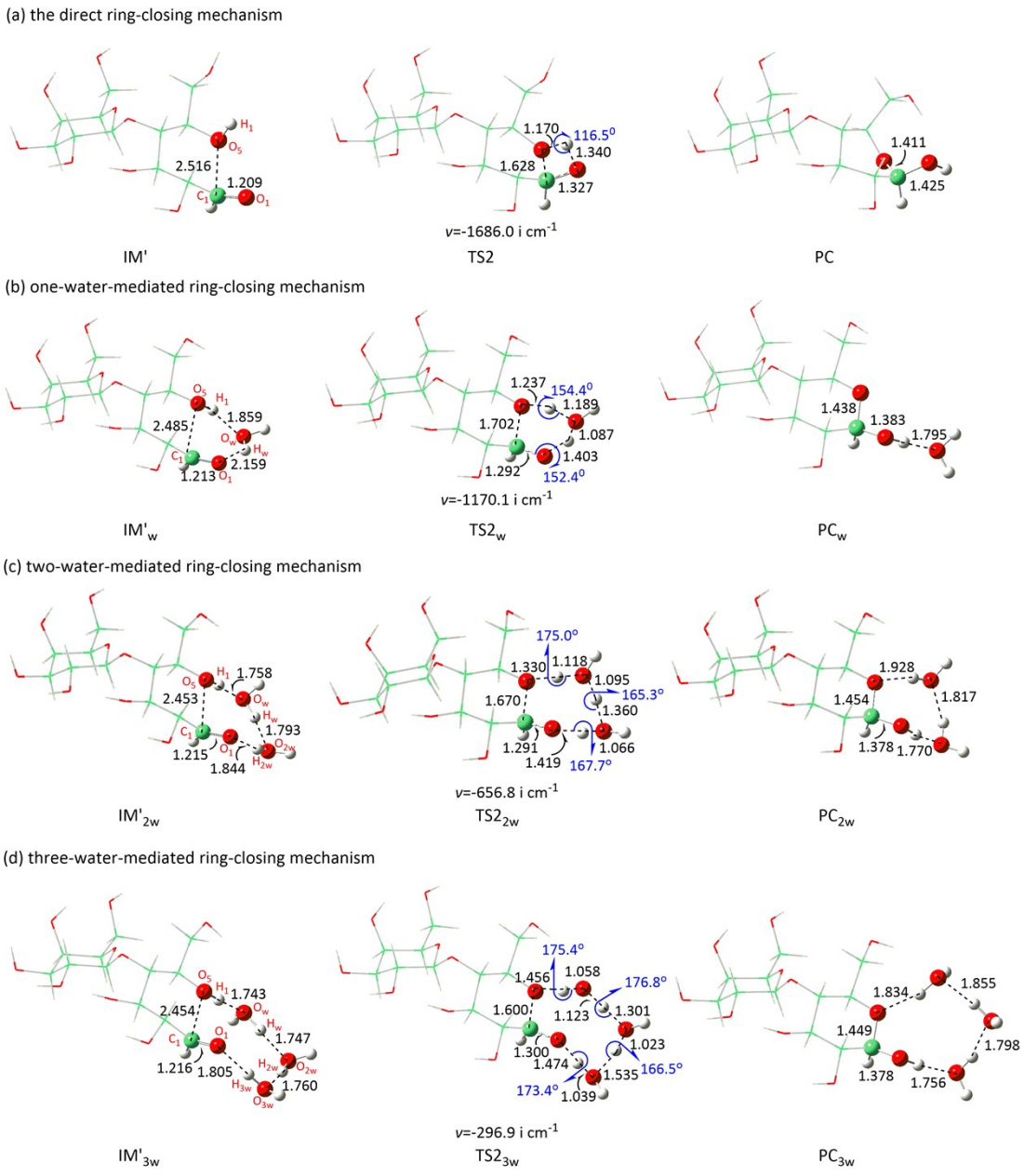

Fig. S2 B3LYP-D3/6-311++G(d,p) optimized structures (Å) of all the stationary points in the solvent-catalyzed ring-closing step of α-lactose (*v* represents for the single imaginary frequency of the transition state).

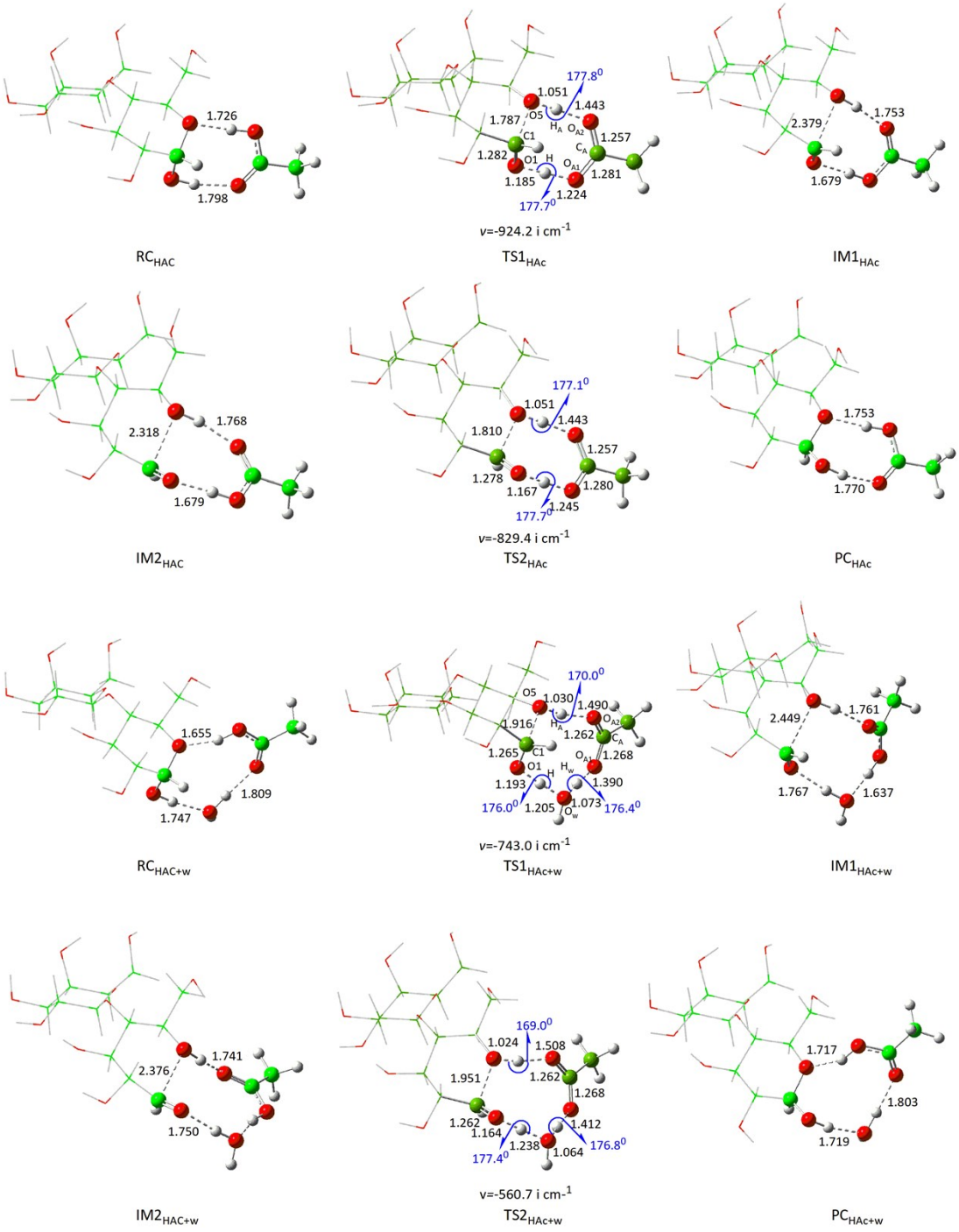

Fig. S3 B3LYP-D3/6-311++G(d,p) optimized structures (Å) of all the stationary points in the HAc-catalyzed mutarotation processes of α-lactose (*v* represents for the single imaginary frequency of the transition state).

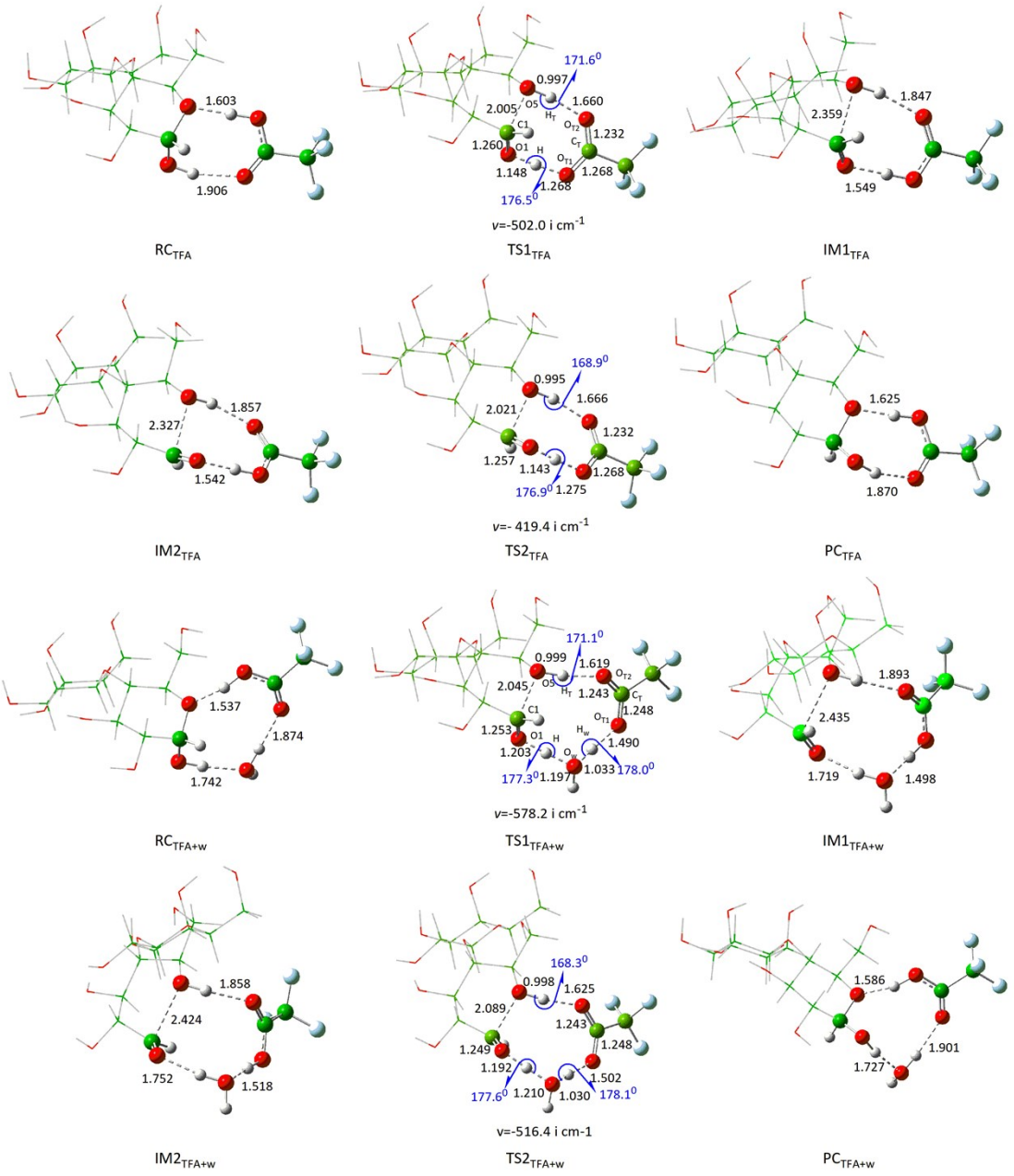

Fig. S4 B3LYP-D3/6-311++G(d,p) optimized structures(Å) of all the stationary points in the TFA-catalyzed mutarotation processes of α-lactose (*v* represents for the single imaginary frequency of the transition state).

Cartesian coordinates of all stationary points

1. Solvent-catalyzed Mechanism

RC

C	2.81988	-1.63901	0.45903
C	1.67744	-1.43125	-0.54132
C	0.78715	-0.2596	-0.12273
C	2.59914	0.79336	1.02956
C	3.58842	-0.33424	0.68351
H	2.08927	-1.20075	-1.52965
H	2.39834	-1.97588	1.41029
H	2.14495	0.5458	2.00059
H	4.26678	-0.46127	1.53728
H	0.28792	-0.4909	0.82727
C	-2.1119	-1.13861	-0.19589
C	-3.60561	-0.93598	0.04815
C	-3.83979	0.31089	0.90579
C	-1.84055	1.37168	0.02606
C	-1.52963	0.13096	-0.82911
H	-4.90599	0.54047	0.9639
H	-4.09182	-0.74987	-0.9182
H	-1.63674	-1.3407	0.7703
H	-1.31454	1.31592	0.98563
H	-1.99177	0.2641	-1.8091
O	-0.13323	-0.00916	-1.14459
O	1.57245	0.91654	0.03535
O	-3.2628	1.44085	0.26397
C	3.24673	2.16691	1.17051
H	2.48968	2.89742	1.4672
H	4.01298	2.1271	1.94597
O	3.9082	2.59378	-0.0311
H	3.23308	2.8338	-0.67762
O	4.34572	-0.09615	-0.50477
H	4.50179	0.86058	-0.57426
O	3.67413	-2.6936	0.01849
H	4.24124	-2.32803	-0.67518
O	0.85043	-2.59724	-0.61108
H	1.42216	-3.35947	-0.77021
O	-1.96477	-2.27234	-1.04454
H	-1.02431	-2.52504	-1.03016
O	-4.19633	-2.06591	0.67487
H	-3.92266	-2.83994	0.16569
O	-3.29925	0.10025	2.18713
H	-3.61624	0.79843	2.77265
C	-1.4704	2.68805	-0.64589
H	-1.67914	3.50622	0.05271
H	-0.40506	2.68862	-0.87347

O	-2.15952	2.89292	-1.87867
H	-3.10547	2.87485	-1.68825

RC_w

C	3.27076	1.41771	-0.30004
C	2.07355	1.28715	0.64721
C	1.06007	0.27313	0.11205
C	2.7727	-0.92055	-1.05799
C	3.87903	0.04518	-0.59867
H	2.41418	0.93417	1.62651
H	2.93217	1.87259	-1.23503
H	2.39416	-0.55207	-2.0231
H	4.60089	0.14583	-1.41963
H	0.63426	0.63363	-0.83338
C	-1.69864	1.53168	0.18726
C	-3.1939	1.55724	-0.11827
C	-3.55059	0.43969	-1.10127
C	-1.75072	-0.96822	-0.25537
C	-1.3154	0.14378	0.7152
H	-4.63328	0.3677	-1.22396
H	-3.74248	1.35097	0.80973
H	-1.16161	1.75278	-0.74174
H	-1.19869	-0.89192	-1.1984
H	-1.82963	-0.01508	1.6645
O	0.07352	0.06884	1.08133
O	1.69764	-0.97957	-0.10962
O	-3.16494	-0.81564	-0.54073
C	3.24831	-2.35324	-1.27679
H	2.41886	-2.95826	-1.65175
H	4.04648	-2.36003	-2.02028
O	3.79778	-2.94268	-0.08739
H	3.07012	-3.13585	0.51645
O	4.55434	-0.37045	0.59051
H	4.5839	-1.34192	0.59509
O	4.23227	2.3214	0.24363
H	4.72342	1.83837	0.92331
O	1.39963	2.54248	0.78236
H	2.0569	3.20872	1.02192
O	-1.43768	2.55507	1.14197
H	-0.4728	2.68486	1.16964
O	-3.60327	2.80838	-0.65181
H	-3.24731	3.48934	-0.06622
O	-2.9173	0.6823	-2.33042
H	-3.32187	0.12381	-3.00489
C	-1.53725	-2.37614	0.29728
H	-1.93817	-3.09358	-0.42841
H	-0.46293	-2.54276	0.3799
O	-2.09555	-2.58993	1.58794
H	-3.06304	-2.66492	1.49717

O	-4.84811	-2.52971	0.96019
H	-4.55193	-2.01477	0.19072
H	-5.30578	-3.29991	0.60447

RC_{2w}

C	-3.49486	1.07699	0.94604
C	-2.49786	1.31932	-0.19178
C	-1.34839	0.31062	-0.13541
C	-2.73628	-1.31161	0.94676
C	-3.96105	-0.38062	0.95832
H	-3.00159	1.20011	-1.15687
H	-3.00627	1.30531	1.89729
H	-2.20099	-1.16178	1.89615
H	-4.51854	-0.5691	1.88506
H	-0.76571	0.46133	0.78261
C	1.27874	1.8118	-0.34293
C	2.80174	1.89839	-0.30663
C	3.38402	0.61524	0.29253
C	1.5279	-0.70268	-0.60345
C	0.8677	0.57575	-1.15107
H	4.47275	0.61141	0.19572
H	3.17353	1.97456	-1.33641
H	0.92196	1.734	0.6896
H	1.14455	-0.93452	0.39592
H	1.19862	0.71811	-2.18136
O	-0.55998	0.46218	-1.28013
O	-1.86164	-1.01658	-0.15196
O	2.95929	-0.49952	-0.5234
C	-3.08192	-2.79386	0.85085
H	-2.1647	-3.38591	0.90402
H	-3.72273	-3.07065	1.68904
O	-3.81435	-3.11503	-0.34276
H	-3.20423	-3.07668	-1.08958
O	-4.82575	-0.54474	-0.16772
H	-4.79941	-1.47939	-0.43289
O	-4.5892	1.98753	0.84444
H	-5.17479	1.65181	0.15103
O	-1.92659	2.62797	-0.09222
H	-2.64997	3.26453	-0.02353
O	0.78896	3.01422	-0.92743
H	-0.16802	3.05193	-0.75066
O	3.24824	3.01598	0.44883
H	2.74822	3.7802	0.13361
O	2.98383	0.47552	1.61553
H	3.58736	-0.15433	2.06898
C	1.31278	-1.91998	-1.4951
H	1.78427	-2.79119	-1.02624
H	0.24365	-2.11297	-1.5749
O	1.79875	-1.73602	-2.82379

H	2.74718	-1.56694	-2.77492
O	4.76516	-1.33944	2.69471
H	4.88543	-1.92727	1.9185
H	4.44972	-1.90194	3.41076
O	4.88917	-2.48894	0.19706
H	4.16707	-1.95606	-0.18584
H	4.69046	-3.40584	-0.0232

RC_{3w}

C	-3.8843	0.83004	0.85405
C	-2.89021	1.13637	-0.27134
C	-1.63592	0.27107	-0.13716
C	-2.86642	-1.45893	0.96857
C	-4.18618	-0.66917	0.91924
H	-3.34818	0.91488	-1.24127
H	-3.44807	1.14991	1.80458
H	-2.37697	-1.22092	1.92469
H	-4.74018	-0.8819	1.84286
H	-1.11016	0.51953	0.79414
C	0.80308	2.06488	-0.32254
C	2.29996	2.35464	-0.22937
C	3.04121	1.17195	0.40084
C	1.368	-0.39508	-0.44691
C	0.57417	0.75449	-1.0896
H	4.122	1.30317	0.29767
H	2.69244	2.46835	-1.24831
H	0.41539	1.97969	0.69859
H	1.01573	-0.57452	0.57499
H	0.92771	0.88541	-2.11419
O	-0.82558	0.46814	-1.25952
O	-1.99871	-1.10503	-0.11783
O	2.75776	0.00073	-0.39109
C	-3.04382	-2.97282	0.91703
H	-2.06831	-3.45667	1.01236
H	-3.67233	-3.29204	1.74948
O	-3.70371	-3.41288	-0.28069
H	-3.08446	-3.32328	-1.01552
O	-5.00292	-0.97158	-0.21406
H	-4.8676	-1.90663	-0.44192
O	-5.0698	1.60697	0.68929
H	-5.59774	1.17632	0.002
O	-2.48047	2.50641	-0.22062
H	-3.27562	3.05374	-0.18126
O	0.19326	3.17616	-0.97095
H	-0.76734	3.10298	-0.82778
O	2.55903	3.53411	0.51956
H	1.98144	4.22092	0.16176
O	2.67279	0.99766	1.72684
H	3.31408	0.37643	2.14186

C	1.28547	-1.72152	-1.19825
H	1.82266	-2.48226	-0.62208
H	0.2363	-2.01322	-1.2489
O	1.77815	-1.66428	-2.5349
H	2.74221	-1.75119	-2.4988
O	5.52819	-2.55232	0.93561
H	5.24952	-2.34011	0.0204
H	5.34997	-3.49142	1.05728
O	4.6005	-1.6316	-1.54246
H	4.07652	-0.90235	-1.14761
H	5.2672	-1.21851	-2.10382
O	4.4758	-0.7822	2.78473
H	5.22043	-0.42988	3.28431
H	4.85873	-1.42446	2.14583

TS1

C	2.90108	-1.6042	0.50297
C	1.74076	-1.44762	-0.48647
C	0.84355	-0.27162	-0.09824
C	2.65682	0.84176	0.99688
C	3.65494	-0.28263	0.66846
H	2.13387	-1.25366	-1.48989
H	2.49854	-1.91182	1.47218
H	2.22196	0.61932	1.98254
H	4.35103	-0.37175	1.51269
H	0.35211	-0.4832	0.86121
C	-2.10008	-1.10626	-0.13081
C	-3.61988	-0.94093	-0.08671
C	-4.06601	0.18352	0.85053
C	-1.6595	1.41869	0.04309
C	-1.47249	0.13504	-0.78494
H	-4.97837	0.6876	0.51444
H	-3.9678	-0.70237	-1.10086
H	-1.72861	-1.25199	0.89092
H	-0.89619	1.46791	0.82249
H	-1.94363	0.26628	-1.76105
O	-0.09018	-0.06523	-1.12123
O	1.61111	0.91872	0.01606
O	-2.94547	1.42844	0.74121
C	3.2868	2.2278	1.08355
H	2.52341	2.95767	1.365
H	4.06179	2.22301	1.85124
O	3.92985	2.62344	-0.13838
H	3.24601	2.84457	-0.78236
O	4.38448	-0.07398	-0.54203
H	4.53359	0.88129	-0.64105
O	3.76177	-2.66257	0.08629
H	4.31564	-2.31462	-0.62688
O	0.92139	-2.6204	-0.49325

H	1.48768	-3.3856	-0.65689
O	-1.85962	-2.27191	-0.90758
H	-0.91197	-2.49553	-0.84644
O	-4.25564	-2.12706	0.37033
H	-3.82855	-2.85681	-0.09999
O	-3.87764	0.07622	2.15423
H	-3.04268	1.02956	1.85105
C	-1.57943	2.68896	-0.7979
H	-1.61155	3.55962	-0.13502
H	-0.63007	2.69932	-1.33567
O	-2.6117	2.75751	-1.77724
H	-3.45222	2.87084	-1.31732

$TS1_w$

C	-3.08825	1.45652	0.73441
C	-2.0049	1.47333	-0.34982
C	-1.00938	0.332	-0.13951
C	-2.66569	-1.00614	0.95093
C	-3.74971	0.07863	0.82158
H	-2.46359	1.34205	-1.3356
H	-2.62486	1.69374	1.6961
H	-2.16833	-0.86031	1.92126
H	-4.37443	0.0394	1.72339
H	-0.47377	0.47653	0.80799
C	1.82468	1.41949	-0.2548
C	3.34793	1.35705	-0.17668
C	3.82417	0.17946	0.67081
C	1.67295	-1.13089	-0.32667
C	1.28316	0.19295	-1.00137
H	4.84946	-0.12567	0.42176
H	3.74972	1.23255	-1.19036
H	1.43239	1.45997	0.76755
H	1.18435	-1.21211	0.65206
H	1.69695	0.20336	-2.01143
O	-0.13363	0.29165	-1.22939
O	-1.69817	-0.91219	-0.10445
O	3.11085	-1.16551	-0.14877
C	-3.20488	-2.43271	0.92895
H	-2.38076	-3.13485	1.07929
H	-3.9225	-2.56165	1.74034
O	-3.90676	-2.74063	-0.28605
H	-3.25717	-2.82974	-0.99427
O	-4.57072	-0.05561	-0.34043
H	-4.65947	-1.00301	-0.53811
O	-4.0397	2.49261	0.49627
H	-4.62925	2.18148	-0.20526
O	-1.26911	2.69968	-0.30601
H	-1.90112	3.43006	-0.32437
O	1.50191	2.62456	-0.94223

H	0.5487	2.78918	-0.8231
O	3.87763	2.54274	0.40704
H	3.39952	3.27813	-0.00078
O	3.47584	0.12392	1.91632
H	3.65558	-1.18467	2.18645
C	1.29789	-2.36099	-1.15394
H	1.55612	-3.26251	-0.58575
H	0.22231	-2.36115	-1.3267
O	1.92651	-2.37508	-2.43283
H	2.88089	-2.35242	-2.29027
O	3.73119	-2.25678	1.88016
H	3.38032	-1.94316	0.78461
H	3.08432	-2.80237	2.34493

$TS1_{2w}$

C	3.40132	1.16524	-0.94123
C	2.39799	1.37971	0.19623
C	1.28039	0.33537	0.14348
C	2.72298	-1.2474	-0.93039
C	3.9159	-0.27583	-0.94666
H	2.90577	1.27949	1.16137
H	2.90476	1.37269	-1.89314
H	2.1853	-1.12255	-1.8821
H	4.47888	-0.45014	-1.87286
H	0.69345	0.46406	-0.77529
C	-1.39471	1.74564	0.35131
C	-2.91744	1.81089	0.30129
C	-3.47757	0.5939	-0.44741
C	-1.54374	-0.79292	0.61654
C	-0.9456	0.51982	1.15493
H	-4.55488	0.4691	-0.25474
H	-3.31568	1.80905	1.32349
H	-1.03293	1.68438	-0.68011
H	-1.15864	-1.00657	-0.38733
H	-1.28336	0.65016	2.18463
O	0.48708	0.46589	1.28651
O	1.83644	-0.97561	0.16457
O	-2.97679	-0.63567	0.55301
C	3.11855	-2.71642	-0.82303
H	2.22213	-3.33976	-0.87442
H	3.77108	-2.9776	-1.65717
O	3.85785	-3.00367	0.37497
H	3.24545	-2.97525	1.1204
O	4.78645	-0.40514	0.17935
H	4.78951	-1.33819	0.45132
O	4.4651	2.11194	-0.84465
H	5.06209	1.79811	-0.1507
O	1.78657	2.66964	0.09246
H	2.49013	3.32785	0.02192

O	-0.93184	2.95526	0.94939
H	0.02199	3.02284	0.76545
O	-3.35473	2.9855	-0.37838
H	-2.81211	3.71063	-0.04015
O	-3.0696	0.40925	-1.66273
H	-3.79725	-0.61679	-2.32826
C	-1.23877	-1.98794	1.5191
H	-1.63366	-2.90182	1.05997
H	-0.15845	-2.09704	1.60678
O	-1.74661	-1.82999	2.84278
H	-2.69722	-1.67609	2.78016
O	-4.36808	-1.46364	-2.63692
H	-4.36384	-2.14215	-1.45278
H	-3.89126	-1.9106	-3.34563
O	-4.31614	-2.43324	-0.39983
H	-3.64265	-1.68088	0.09399
H	-3.99008	-3.33733	-0.30392

$TS1_{3w}$

C	3.73977	0.86844	-1.08364
C	2.82744	1.22298	0.09589
C	1.60147	0.30839	0.13289
C	2.79796	-1.45212	-0.95751
C	4.08889	-0.62207	-1.07299
H	3.37143	1.09092	1.0374
H	3.21889	1.10833	-2.01487
H	2.22093	-1.28972	-1.88017
H	4.57322	-0.88217	-2.02332
H	0.98913	0.46867	-0.76384
C	-0.90738	1.98451	0.38468
C	-2.41802	2.18767	0.38551
C	-3.11057	0.95768	-0.23182
C	-1.30912	-0.49725	0.8156
C	-0.54017	0.76719	1.23994
H	-4.19504	0.9889	-0.02885
H	-2.76854	2.31032	1.41826
H	-0.6018	1.83072	-0.65473
H	-1.01271	-0.80638	-0.19339
H	-0.8019	0.99191	2.27535
O	0.88529	0.56477	1.30395
O	2.01601	-1.05389	0.17668
O	-2.71466	-0.17838	0.81472
C	3.03253	-2.95355	-0.82941
H	2.07004	-3.47122	-0.80686
H	3.59642	-3.30712	-1.69367
O	3.81013	-3.29607	0.32906
H	3.2546	-3.17897	1.10949
O	5.00491	-0.81934	0.00622
H	4.92944	-1.74253	0.30001

O	4.90637	1.69025	-1.06916
H	5.50164	1.32499	-0.39934
O	2.35838	2.57018	-0.01827
H	3.12516	3.14206	-0.15288
O	-0.30325	3.17665	0.88849
H	0.64423	3.13585	0.66954
O	-2.77678	3.33909	-0.37675
H	-2.17012	4.04228	-0.10968
O	-2.75855	0.64919	-1.44925
H	-3.76062	0.01432	-2.28599
C	-1.08036	-1.67369	1.76089
H	-1.65826	-2.53504	1.40774
H	-0.02395	-1.93878	1.73881
O	-1.39513	-1.38164	3.12384
H	-2.32528	-1.13304	3.17654
O	-5.39935	-2.34598	-1.43079
H	-4.85212	-2.18772	-0.26275
H	-5.21322	-3.20775	-1.82282
O	-4.37602	-2.02175	0.7419
H	-3.65184	-1.23926	0.752
H	-5.04607	-1.85228	1.41773
O	-4.45792	-0.49381	-2.88456
H	-5.08243	0.1555	-3.22462
H	-5.06144	-1.61597	-2.07376

IM1

C	2.69612	-1.77928	0.40779
C	1.55745	-1.47122	-0.57082
C	0.73032	-0.27531	-0.09596
C	2.60132	0.63242	1.08833
C	3.53057	-0.52619	0.6856
H	1.96987	-1.22267	-1.55434
H	2.26385	-2.13858	1.34562
H	2.13901	0.36616	2.05039
H	4.20594	-0.72669	1.52743
H	0.22621	-0.51975	0.84844
C	-2.22061	-0.92876	-0.17828
C	-3.74317	-0.82295	0.03749
C	-4.12305	-0.14775	1.36085
C	-1.66552	1.62774	0.07244
C	-1.55668	0.33968	-0.76147
H	-5.05577	0.44152	1.3429
H	-4.20779	-0.27913	-0.79158
H	-1.76758	-1.1964	0.78181
H	-1.21219	1.48246	1.05993
H	-2.01702	0.52821	-1.73331
O	-0.18401	0.05543	-1.10204
O	1.57922	0.84945	0.10494
O	-3.07453	1.88955	0.21388

C	3.31584	1.96572	1.28396
H	2.59619	2.71812	1.61665
H	4.08283	1.85589	2.05177
O	3.99098	2.41174	0.09688
H	3.32476	2.71172	-0.53364
O	4.29278	-0.27253	-0.49627
H	4.49499	0.67767	-0.52472
O	3.49401	-2.85275	-0.08854
H	4.07455	-2.48347	-0.76904
O	0.66992	-2.58889	-0.67582
H	1.19086	-3.37058	-0.90061
O	-2.04678	-2.00327	-1.10461
H	-1.11862	-2.30097	-1.06164
O	-4.31237	-2.13256	0.13189
H	-3.76097	-2.69062	-0.4402
O	-3.51479	-0.32378	2.39209
H	-3.19881	2.56183	0.89533
C	-0.99838	2.83194	-0.59866
H	-1.08458	3.69328	0.07656
H	0.0578	2.63064	-0.76421
O	-1.5729	3.13316	-1.86905
H	-2.52089	3.26077	-1.73804

IM1$_w$

C	-3.00113	1.53121	0.78005
C	-1.92805	1.51644	-0.31432
C	-0.97415	0.3353	-0.12789
C	-2.67532	-0.9474	0.96506
C	-3.71628	0.18067	0.85991
H	-2.40059	1.41486	-1.29697
H	-2.52029	1.73978	1.7397
H	-2.1622	-0.83194	1.93123
H	-4.33243	0.15628	1.7681
H	-0.4247	0.44578	0.81676
C	1.90745	1.29914	-0.30348
C	3.44909	1.33309	-0.2638
C	4.05654	0.48686	0.8567
C	1.57337	-1.30375	-0.37425
C	1.30262	0.06758	-1.01779
H	5.00251	-0.02147	0.60905
H	3.85485	0.99356	-1.22339
H	1.5418	1.36867	0.72684
H	1.14366	-1.33747	0.63345
H	1.70085	0.05253	-2.03458
O	-0.11092	0.27801	-1.22689
O	-1.71612	-0.87942	-0.09969
O	2.9975	-1.46714	-0.30086
C	-3.27136	-2.3509	0.93396
H	-2.47442	-3.08735	1.06574

H	-3.98348	-2.46005	1.75302
O	-4.00037	-2.61617	-0.27508
H	-3.36396	-2.71974	-0.99324
O	-4.5546	0.09331	-0.29437
H	-4.68869	-0.84729	-0.49876
O	-3.91251	2.60663	0.56011
H	-4.52193	2.32401	-0.13648
O	-1.14539	2.71297	-0.2632
H	-1.74528	3.46963	-0.29054
O	1.53819	2.47764	-1.02232
H	0.59589	2.66373	-0.84961
O	3.89811	2.66376	0.00532
H	3.23744	3.24094	-0.41095
O	3.60429	0.4475	1.98274
H	3.72083	-1.57005	2.58884
C	0.99661	-2.46783	-1.18751
H	1.13429	-3.39061	-0.61
H	-0.06744	-2.32387	-1.36231
O	1.62382	-2.58222	-2.46455
H	2.57656	-2.6126	-2.30648
O	3.71177	-2.4519	2.18414
H	3.20736	-2.00603	0.48984
H	3.183	-3.0076	2.768

IM1$_{2w}$

C	-3.29146	1.23944	1.06041
C	-2.32297	1.44962	-0.10777
C	-1.24345	0.36531	-0.1277
C	-2.70241	-1.19504	0.95717
C	-3.85683	-0.18263	1.04896
H	-2.86785	1.39908	-1.05622
H	-2.75243	1.40446	1.99739
H	-2.1228	-1.11846	1.88912
H	-4.3885	-0.36277	1.99235
H	-0.61974	0.44456	0.77282
C	1.50147	1.62525	-0.41754
C	3.0337	1.79547	-0.48112
C	3.78322	0.89855	0.50497
C	1.41296	-0.96946	-0.78437
C	0.95227	0.42954	-1.22785
H	4.73371	0.47369	0.14956
H	3.39323	1.59072	-1.49501
H	1.21569	1.5438	0.63689
H	1.07371	-1.17134	0.23885
H	1.25501	0.57383	-2.26705
O	-0.48755	0.51131	-1.2948
O	-1.85095	-0.92201	-0.16528
O	2.84421	-0.97055	-0.83612
C	-3.15469	-2.64559	0.82438

H	-2.27952	-3.30048	0.82061
H	-3.78133	-2.90882	1.67754
O	-3.95243	-2.87148	-0.34874
H	-3.3714	-2.83888	-1.11872
O	-4.77539	-0.24853	-0.0439
H	-4.82796	-1.17332	-0.33801
O	-4.32367	2.22413	1.0267
H	-4.95902	1.9452	0.35215
O	-1.65807	2.7112	0.01241
H	-2.32917	3.40005	0.10265
O	0.97406	2.83624	-0.96251
H	0.03686	2.91021	-0.70118
O	3.39076	3.12692	-0.1021
H	2.64897	3.68061	-0.39554
O	3.4266	0.75655	1.65917
H	4.19378	-0.59579	2.65293
C	0.88352	-2.08086	-1.69842
H	1.17392	-3.04811	-1.26891
H	-0.20235	-2.04134	-1.75659
O	1.38392	-1.95729	-3.02946
H	2.3443	-1.87466	-2.96239
O	4.56209	-1.45312	2.94769
H	4.13363	-2.54744	1.59588
H	4.18688	-1.6172	3.82003
O	3.91141	-2.95297	0.72842
H	3.18539	-1.72578	-0.30195
H	3.39507	-3.74256	0.92415

$IM1_{3w}$

C	3.53454	0.87979	-1.36545
C	2.71211	1.30709	-0.14592
C	1.54467	0.34677	0.0926
C	2.73313	-1.45678	-0.93836
C	3.96194	-0.58494	-1.2477
H	3.34263	1.29757	0.74937
H	2.92278	1.00489	-2.26302
H	2.06848	-1.41219	-1.81413
H	4.3758	-0.91425	-2.20963
H	0.84505	0.3928	-0.75292
C	-1.02615	1.91315	0.48256
C	-2.52519	2.23601	0.6587
C	-3.43363	1.34724	-0.19298
C	-1.1483	-0.62548	1.12206
C	-0.51525	0.75429	1.36619
H	-4.38934	1.04768	0.26145
H	-2.81269	2.13994	1.71045
H	-0.85066	1.70176	-0.57751
H	-0.90526	-0.97837	0.11208
H	-0.69942	1.03438	2.40538

O	0.92509	0.69018	1.29765
O	2.03261	-0.98468	0.22164
O	-2.56362	-0.46125	1.25895
C	3.05732	-2.92667	-0.69297
H	2.12936	-3.48202	-0.53427
H	3.5612	-3.33632	-1.56946
O	3.95051	-3.1205	0.41523
H	3.4595	-2.95774	1.22993
O	4.97679	-0.63479	-0.24235
H	4.97547	-1.52732	0.14221
O	4.65297	1.74991	-1.53392
H	5.32367	1.47663	-0.89204
O	2.15798	2.61147	-0.34553
H	2.87631	3.21319	-0.57998
O	-0.33941	3.11205	0.84772
H	0.56875	3.0652	0.49412
O	-2.79431	3.56513	0.20543
H	-1.97001	4.05549	0.35853
O	-3.18716	1.09571	-1.35742
H	-4.3275	0.22045	-2.45269
C	-0.66211	-1.6773	2.12603
H	-1.09446	-2.64552	1.84574
H	0.42273	-1.75874	2.0917
O	-1.01683	-1.34292	3.46839
H	-1.96667	-1.1676	3.47612
O	-5.14172	-2.81703	-1.92289
H	-4.267	-2.80531	-0.40972
H	-4.86538	-3.47244	-2.57266
O	-3.76554	-2.76384	0.43794
H	-3.01498	-1.27714	0.93615
H	-4.32305	-3.18845	1.09902
O	-4.88887	-0.32998	-3.03821
H	-5.68843	0.18285	-3.19959
H	-5.08329	-1.94405	-2.37425

TS_R

C	-2.44382	1.7603	0.
C	-3.52464	2.16647	-1.00263
C	-4.28127	3.39616	-0.50978
C	-2.38052	4.1569	0.71679
C	-1.52953	2.94395	0.31352
H	-3.06555	2.41752	-1.96396
H	-2.92812	1.4238	0.92027
H	-2.87543	3.91351	1.66778
H	-0.88692	2.68493	1.16419
H	-4.80271	3.16174	0.42698
C	-7.21752	2.83851	-0.6651
C	-8.74774	2.92174	-0.36414
C	-8.9994	3.34951	1.08445

C	-6.58567	5.35791	-0.20932
C	-6.5253	4.13239	-1.14153
H	-9.22959	4.41147	1.24099
H	-9.21859	3.64925	-1.03417
H	-6.72741	2.45553	0.23614
H	-6.20872	5.1038	0.78463
H	-6.98063	4.41075	-2.09346
O	-5.16679	3.80911	-1.50718
O	-3.36656	4.45777	-0.2781
O	-7.94718	5.75867	-0.04398
C	-1.58	5.43514	0.92424
H	-2.2441	6.226	1.28151
H	-0.80427	5.26479	1.67107
O	-0.90822	5.85197	-0.27463
H	-1.57998	6.15122	-0.90004
O	-0.72927	3.16023	-0.84957
H	-0.49306	4.10248	-0.88077
O	-1.71462	0.63883	-0.49301
H	-1.09446	0.97639	-1.15472
O	-4.47565	1.11166	-1.16697
H	-3.99301	0.30025	-1.37082
O	-7.08826	1.86848	-1.70426
H	-6.18347	1.50363	-1.65825
O	-9.32663	1.63997	-0.54001
H	-8.74183	1.17929	-1.16428
O	-8.94479	2.5713	2.00976
H	-8.16373	6.29872	-0.81814
C	-5.78579	6.53904	-0.74868
H	-5.81161	7.33972	-0.00356
H	-4.7529	6.25437	-0.94172
O	-6.44631	6.95863	-1.95435
H	-6.15782	7.84974	-2.17453

IM2

C	-2.87632	-1.70652	-0.49573
C	-1.70535	-1.50028	0.47224
C	-0.8391	-0.31445	0.04697
C	-2.68938	0.73274	-1.04983
C	-3.66003	-0.40541	-0.68756
H	-2.08729	-1.29368	1.47744
H	-2.48016	-2.03281	-1.4614
H	-2.2566	0.49752	-2.03347
H	-4.36086	-0.53065	-1.52321
H	-0.36111	-0.53214	-0.91818
C	2.15024	-0.99827	0.05881
C	3.69442	-0.94306	-0.00695
C	4.2772	-0.21262	-1.21566
C	1.51698	1.53415	-0.15662
C	1.4665	0.24297	0.6857

H	3.6772	-0.26112	-2.14198
H	4.10176	-0.50529	0.91193
H	1.7684	-1.17491	-0.95582
H	0.90306	1.41458	-1.05181
H	1.9422	0.42854	1.65126
O	0.10636	-0.0783	1.05089
O	-1.64007	0.85429	-0.07872
O	2.85042	1.77124	-0.61299
C	-3.35025	2.1026	-1.16253
H	-2.60596	2.84152	-1.4702
H	-4.13412	2.06382	-1.92016
O	-3.98653	2.51358	0.05807
H	-3.29851	2.75712	0.68947
O	-4.38521	-0.18319	0.52357
H	-4.55113	0.77118	0.60273
O	-3.7104	-2.76941	-0.03844
H	-4.26202	-2.41161	0.67161
O	-0.85756	-2.65232	0.49106
H	-1.39413	-3.42617	0.70518
O	1.87744	-2.13941	0.87406
H	0.93247	-2.37387	0.80485
O	4.20142	-2.2728	-0.17989
H	3.55058	-2.85152	0.25088
O	5.39227	0.25688	-1.21326
H	3.30813	2.24622	0.09765
C	1.01844	2.7529	0.61438
H	0.94326	3.60017	-0.07374
H	0.03731	2.55249	1.04819
O	1.99426	3.02339	1.63323
H	1.86821	3.92047	1.95873

IM2$_w$

C	-3.17095	-1.46153	-0.78856
C	-2.08261	-1.47036	0.29064
C	-1.09285	-0.32433	0.07744
C	-2.76103	1.00201	-1.01139
C	-3.83948	-0.08722	-0.87668
H	-2.53721	-1.34247	1.27862
H	-2.7107	-1.69937	-1.75153
H	-2.26433	0.85577	-1.98192
H	-4.46755	-0.05317	-1.77632
H	-0.55959	-0.46466	-0.8724
C	1.774	-1.36143	0.23323
C	3.31538	-1.4623	0.17047
C	3.9406	-0.65174	-0.9594
C	1.49881	1.24279	0.26655
C	1.19909	-0.10822	0.93799
H	3.29604	-0.48625	-1.84203
H	3.76598	-1.16608	1.12366

H	1.3935	-1.42406	-0.79498
H	1.04928	1.28102	-0.73257
H	1.61022	-0.08348	1.94915
O	-0.2144	-0.28609	1.1654
O	-1.79217	0.91446	0.04326
O	2.92376	1.31353	0.17278
C	-3.3063	2.42631	-0.99248
H	-2.48534	3.13151	-1.14533
H	-4.02527	2.5499	-1.80348
O	-4.0083	2.73437	0.22256
H	-3.35806	2.83247	0.92898
O	-4.65697	0.04586	0.28807
H	-4.74987	0.99341	0.48328
O	-4.1165	-2.50111	-0.54252
H	-4.70561	-2.18934	0.1591
O	-1.33819	-2.69126	0.24285
H	-1.95941	-3.42929	0.29223
O	1.36702	-2.52616	0.95327
H	0.41511	-2.67498	0.79632
O	3.67884	-2.81014	-0.15101
H	2.97715	-3.36106	0.23349
O	5.10593	-0.31517	-0.97293
H	5.01816	1.67367	-1.81077
C	0.98668	2.43918	1.07478
H	1.17053	3.35091	0.49234
H	-0.08389	2.35011	1.24862
O	1.6157	2.52923	2.35282
H	2.56967	2.51728	2.20139
O	4.39982	2.41778	-1.88055
H	3.21715	1.92197	-0.53431
H	4.9396	3.21479	-1.82898

$IM2_{2w}$

C	3.50794	1.21217	-1.04034
C	2.49285	1.43354	0.08542
C	1.39952	0.36353	0.05946
C	2.87623	-1.21253	-0.9766
C	4.04969	-0.21869	-1.01124
H	2.99613	1.3789	1.05623
H	3.01288	1.38939	-1.99902
H	2.33694	-1.11898	-1.93089
H	4.61998	-0.40265	-1.93106
H	0.81085	0.45937	-0.86338
C	-1.38544	1.61016	0.2788
C	-2.91235	1.82854	0.37916
C	-3.73735	0.97477	-0.57349
C	-1.23934	-0.98356	0.57731
C	-0.83173	0.40896	1.08289
H	-3.24637	0.68597	-1.51775

H	-3.25981	1.66549	1.40538
H	-1.12289	1.51183	-0.78314
H	-0.7788	-1.17455	-0.39877
H	-1.17115	0.51964	2.11482
O	0.60277	0.51747	1.19853
O	1.98358	-0.93328	0.112
O	-2.66303	-0.97603	0.45617
C	3.29939	-2.67114	-0.83759
H	2.41483	-3.31206	-0.87532
H	3.95628	-2.93736	-1.66675
O	4.04467	-2.91876	0.36538
H	3.43176	-2.89173	1.11042
O	4.91697	-0.30521	0.12128
H	4.94158	-1.23258	0.41104
O	4.55298	2.18006	-0.95757
H	5.15348	1.88976	-0.25644
O	1.84373	2.70008	-0.06392
H	2.52019	3.38812	-0.10511
O	-0.82305	2.81726	0.79483
H	0.12325	2.85861	0.55844
O	-3.22374	3.16285	-0.0393
H	-2.43826	3.68871	0.18576
O	-4.91978	0.75654	-0.39286
H	-5.67953	-0.51827	-1.4877
C	-0.81952	-2.10285	1.53736
H	-1.04399	-3.0675	1.06473
H	0.25079	-2.05483	1.7308
O	-1.48224	-1.99878	2.79696
H	-2.42742	-1.92124	2.61194
O	-3.67521	-2.84407	-1.26956
H	-2.95888	-1.70699	-0.13585
H	-3.91836	-3.70759	-0.91777
O	-5.84008	-1.31353	-2.03575
H	-6.75105	-1.57581	-1.86299
H	-4.51237	-2.42794	-1.57391

$IM2_{3w}$

C	3.83019	0.93952	-1.26385
C	2.89834	1.34469	-0.11618
C	1.73611	0.36083	0.02499
C	3.03593	-1.41354	-0.9184
C	4.2715	-0.51897	-1.11969
H	3.45168	1.34918	0.82871
H	3.29453	1.06135	-2.20929
H	2.4446	-1.3723	-1.84527
H	4.77016	-0.83439	-2.04532
H	1.10269	0.40404	-0.87168
C	-0.95328	1.82207	0.26837
C	-2.44485	2.17028	0.4747

C	-3.42668	1.31908	-0.31773
C	-0.94487	-0.73555	0.79685
C	-0.42471	0.66544	1.15085
H	-3.07359	0.93763	-1.28945
H	-2.70646	2.12568	1.53792
H	-0.79259	1.59843	-0.79492
H	-0.5248	-1.05271	-0.16461
H	-0.69423	0.89088	2.18472
O	1.01832	0.68617	1.18047
O	2.23611	-0.96194	0.18408
O	-2.36819	-0.64706	0.70099
C	3.36275	-2.88005	-0.65719
H	2.43355	-3.4493	-0.57207
H	3.93731	-3.27686	-1.49529
O	4.17243	-3.0685	0.51453
H	3.61812	-2.92188	1.29077
O	5.19853	-0.55913	-0.03253
H	5.18704	-1.45758	0.33795
O	4.94334	1.82921	-1.32979
H	5.56193	1.55995	-0.63605
O	2.33038	2.63471	-0.36265
H	3.04883	3.26407	-0.50559
O	-0.26488	3.02582	0.6101
H	0.66307	2.96637	0.31249
O	-2.69589	3.48512	-0.03725
H	-1.85315	3.95929	0.05949
O	-4.59244	1.21403	0.01202
H	-5.8625	0.41472	-0.99118
C	-0.57091	-1.78199	1.85269
H	-0.87315	-2.77024	1.485
H	0.50587	-1.78825	2.01431
O	-1.18562	-1.50998	3.11214
H	-2.13069	-1.39766	2.94548
O	-3.2347	-2.81608	-0.71133
H	-2.69978	-1.41686	0.18016
H	-2.6947	-3.07275	-1.46688
O	-6.51068	-0.07113	-1.54362
H	-7.38097	0.21008	-1.24043
H	-4.16551	-2.8028	-1.03624
O	-5.81883	-2.7202	-1.59674
H	-6.45655	-3.25295	-1.10927
H	-6.1509	-1.7942	-1.55934

TS2

C	3.00494	-1.55987	0.47272
C	1.81379	-1.43168	-0.48359
C	0.88694	-0.29411	-0.05374
C	2.68895	0.87062	1.0039
C	3.71628	-0.21473	0.63738

H	2.17253	-1.21002	-1.49423
H	2.63973	-1.89488	1.44761
H	2.28828	0.62251	1.99785
H	4.43525	-0.28968	1.46354
H	0.43441	-0.53384	0.91793
C	-2.0278	-1.21192	0.01042
C	-3.5493	-1.10576	0.11711
C	-4.01166	0.04979	1.00703
C	-1.66539	1.30914	0.18792
C	-1.46146	0.04729	-0.66817
H	-3.93613	-0.19626	2.07249
H	-3.96048	-0.94304	-0.88699
H	-1.61158	-1.33462	1.01976
H	-0.94164	1.32366	1.00553
H	-1.96869	0.17176	-1.62619
O	-0.08517	-0.11179	-1.04541
O	1.61542	0.92136	0.05171
O	-2.98156	1.29592	0.81222
C	3.2723	2.27685	1.09116
H	2.4911	2.97621	1.39983
H	4.06586	2.29084	1.83954
O	3.87044	2.70826	-0.14144
H	3.16323	2.91225	-0.76551
O	4.40927	0.03291	-0.58745
H	4.52434	0.99365	-0.67841
O	3.89085	-2.58125	0.01814
H	4.41109	-2.20422	-0.70549
O	1.03712	-2.63289	-0.48594
H	1.62621	-3.37579	-0.67046
O	-1.77174	-2.37667	-0.76193
H	-0.81475	-2.56468	-0.73708
O	-4.10095	-2.289	0.68568
H	-3.67862	-3.03309	0.23466
O	-5.04568	0.78089	0.60872
H	-4.01846	1.60867	0.3695
C	-1.53111	2.60894	-0.58561
H	-1.66177	3.44911	0.10422
H	-0.52076	2.65134	-1.00374
O	-2.5238	2.63183	-1.61086
H	-2.47166	3.4762	-2.07095

$TS2_w$

C	-3.25681	1.40274	0.68332
C	-2.14828	1.40046	-0.3747
C	-1.12745	0.29791	-0.08924
C	-2.77408	-1.03465	1.0238
C	-3.88284	0.01192	0.81608
H	-2.57899	1.21103	-1.36363
H	-2.82399	1.69569	1.64398

H	-2.30632	-0.83037	1.99826
H	-4.53157	-0.00429	1.70144
H	-0.61728	0.49984	0.86172
C	1.67088	1.48166	-0.21956
C	3.19051	1.50475	-0.03309
C	3.64998	0.3652	0.87098
C	1.62434	-1.07096	-0.13299
C	1.1861	0.19034	-0.89748
H	3.02335	0.27115	1.77411
H	3.69065	1.40148	-1.00411
H	1.21933	1.57495	0.77705
H	1.15652	-1.11159	0.85915
H	1.62229	0.14617	-1.89668
O	-0.22684	0.23151	-1.15744
O	-1.78244	-0.96239	-0.01109
O	3.05222	-0.97459	0.00706
C	-3.27354	-2.4754	1.05666
H	-2.43389	-3.1459	1.25706
H	-4.00506	-2.58676	1.85818
O	-3.93991	-2.85952	-0.15671
H	-3.27265	-2.96903	-0.84532
O	-4.66584	-0.1982	-0.36081
H	-4.72709	-1.15603	-0.51365
O	-4.22994	2.39996	0.37598
H	-4.79352	2.04101	-0.32402
O	-1.44673	2.64763	-0.37227
H	-2.09799	3.35771	-0.44263
O	1.33308	2.62926	-0.9925
H	0.37288	2.77169	-0.90482
O	3.58093	2.72527	0.59358
H	3.06895	3.42437	0.16346
O	4.91838	0.16283	1.01682
H	5.0078	-1.21056	1.29273
C	1.29333	-2.37138	-0.86358
H	1.64211	-3.21518	-0.25687
H	0.21153	-2.44855	-0.9667
O	1.83796	-2.43439	-2.17952
H	2.79983	-2.41104	-2.11274
O	4.63091	-2.22915	1.24698
H	3.72615	-1.84159	0.57849
H	5.2398	-2.78547	0.74349

$TS2_{2w}$

C	3.58128	1.17469	-0.89939
C	2.54839	1.35379	0.21774
C	1.42052	0.32777	0.08879
C	2.86927	-1.22569	-1.01577
C	4.07551	-0.27238	-0.95539
H	3.02679	1.20732	1.19191

H	3.1153	1.43199	-1.85461
H	2.35809	-1.04897	-1.97395
H	4.66266	-0.41355	-1.8721
H	0.86339	0.50498	-0.84059
C	-1.26702	1.72501	0.27673
C	-2.7883	1.83164	0.20861
C	-3.41348	0.65234	-0.5395
C	-1.41193	-0.81013	0.43744
C	-0.83254	0.47572	1.04865
H	-2.90572	0.4645	-1.5021
H	-3.20705	1.85436	1.22286
H	-0.89275	1.68245	-0.75472
H	-0.9862	-0.98637	-0.55938
H	-1.19794	0.56301	2.07319
O	0.59623	0.42314	1.2139
O	1.95811	-0.99014	0.06767
O	-2.84076	-0.6508	0.33409
C	3.24058	-2.70408	-0.96782
H	2.33641	-3.30991	-1.06869
H	3.90798	-2.93626	-1.79877
O	3.94764	-3.05913	0.2313
H	3.31754	-3.06411	0.96222
O	4.91081	-0.46518	0.1881
H	4.89459	-1.40983	0.41604
O	4.65453	2.09991	-0.73035
H	5.22736	1.74665	-0.035
O	1.95304	2.65351	0.15063
H	2.66297	3.30838	0.13561
O	-0.79012	2.91592	0.89801
H	0.17123	2.96522	0.74653
O	-3.15547	3.01702	-0.49763
H	-2.563	3.71243	-0.17996
O	-4.70373	0.59436	-0.54235
H	-5.26716	-0.36967	-1.41823
C	-1.13761	-2.04541	1.29705
H	-1.53868	-2.93126	0.79112
H	-0.06086	-2.17271	1.4013
O	-1.6708	-1.93208	2.61518
H	-2.61839	-1.76562	2.53981
O	-4.00084	-2.56991	-0.64439
H	-3.45683	-1.72387	-0.15634
H	-4.40844	-3.13842	0.02274
O	-5.54377	-1.23593	-1.97519
H	-6.49334	-1.37344	-1.88117
H	-4.77499	-2.1025	-1.26234

$TS2_{3w}$

C	3.93505	0.98951	-1.03871
C	2.96886	1.26932	0.11791

C	1.76998	0.32013	0.07282	O	4.05674	-3.23351	0.1895
C	3.05227	-1.3564	-1.05366	H	3.46506	-3.16824	0.9492
C	4.32354	-0.49069	-1.07832	O	5.19955	-0.71382	0.02867
H	3.48116	1.11743	1.0739	H	5.13445	-1.65012	0.28038
H	3.44371	1.25635	-1.97846	O	5.07747	1.83922	-0.94356
H	2.50717	-1.16506	-1.99007	H	5.65764	1.46021	-0.26816
H	4.85305	-0.69578	-2.01789	O	2.45895	2.604	0.03727
H	1.1805	0.50948	-0.83387	H	3.20894	3.20917	-0.02776
C	-0.82385	1.87814	0.33622	O	-0.2427	3.06646	0.86981
C	-2.3375	2.05391	0.36559	H	0.71107	3.04658	0.67232
C	-3.07351	0.86185	-0.26584	O	-2.70161	3.21837	-0.3782
C	-1.10562	-0.62856	0.60304	H	-2.06493	3.90385	-0.13435
C	-0.41874	0.63969	1.13581	O	-4.36895	0.87622	-0.15
H	-2.67884	0.66715	-1.28238	H	-5.25353	0.50265	-1.26952
H	-2.67835	2.1525	1.40469	C	-0.86656	-1.83727	1.50997
H	-0.52133	1.76948	-0.71392	H	-1.31146	-2.72974	1.05584
H	-0.72764	-0.86981	-0.40013	H	0.2058	-2.00393	1.60379
H	-0.72329	0.78709	2.17331	O	-1.37358	-1.64272	2.82913
O	1.01146	0.50304	1.23213	H	-2.30973	-1.41947	2.75381
O	2.21703	-1.03112	0.06621	O	-3.78844	-2.44788	-0.19145
O	-2.52833	-0.40373	0.5473	H	-3.28858	-1.55955	0.09232
C	3.32082	-2.85596	-0.98488	H	-3.26422	-2.91884	-0.85351
H	2.3725	-3.39776	-1.02905	O	-5.90389	0.14161	-1.99614
H	3.9305	-3.1536	-1.83905	H	-6.66226	0.73419	-2.02789

H	-4.84205	-2.32545	-0.56235
O	-6.04241	-2.21538	-1.05384
H	-6.73509	-2.32991	-0.39171
H	-6.12915	-1.27696	-1.45363

PC

C	-3.03747	-1.46278	-0.54387
C	-1.86101	-1.37588	0.43361
C	-0.94562	-0.20036	0.08331
C	-2.76408	1.0012	-0.9092
C	-3.77425	-0.12401	-0.62402
H	-2.23654	-1.2155	1.44981
H	-2.65472	-1.72227	-1.53492
H	-2.35491	0.82783	-1.91553
H	-4.48541	-0.15714	-1.45959
H	-0.48249	-0.36591	-0.89891
C	1.93182	-1.23706	0.06218
C	3.43416	-1.06397	-0.13296
C	3.71753	0.13922	-1.04723
C	1.71679	1.28648	-0.14329
C	1.40282	0.04116	0.72103
H	3.9787	-0.22225	-2.04281
H	3.89247	-0.88375	0.84757
H	1.46688	-1.39642	-0.91804
H	0.80023	1.61292	-0.63809
H	1.89903	0.13555	1.68836
O	0.01565	-0.05738	1.088
O	-1.69696	1.0078	0.05079
O	2.59269	0.96627	-1.25502
C	-3.37115	2.40016	-0.90152
H	-2.60313	3.1315	-1.16617
H	-4.17014	2.45218	-1.64235
O	-3.96693	2.73747	0.36156
H	-3.257	2.894	0.99641
O	-4.48182	0.02957	0.60787
H	-4.60053	0.98059	0.76917
O	-3.90748	-2.53128	-0.17245
H	-4.4435	-2.21715	0.56947
O	-1.07231	-2.56874	0.38129
H	-1.6659	-3.32309	0.49109
O	1.73155	-2.38037	0.88069
H	0.7818	-2.59537	0.84846
O	4.02416	-2.21232	-0.73349
H	3.73262	-2.97676	-0.21915
O	4.81883	0.85824	-0.49749
H	5.17993	1.43745	-1.18113
C	2.22406	2.47697	0.67326
H	2.44044	3.30242	-0.01525
H	1.4207	2.79595	1.34209

O	3.34884	2.19219	1.4983
H	4.07005	1.88673	0.92142

PC_w

C	-3.30952	-1.30609	-0.86181
C	-2.26795	-1.37561	0.26026
C	-1.21761	-0.27589	0.09611
C	-2.77491	1.13805	-1.04238
C	-3.90813	0.09951	-0.96143
H	-2.75662	-1.23067	1.22968
H	-2.82296	-1.55719	-1.80845
H	-2.24932	0.97729	-1.99548
H	-4.49748	0.17158	-1.88476
H	-0.65544	-0.43463	-0.83316
C	1.54807	-1.50441	0.29263
C	3.07137	-1.48424	0.18038
C	3.5299	-0.17058	-0.45234
C	1.58403	1.01775	0.38624
C	1.04655	-0.26608	1.04361
H	3.14335	-0.08856	-1.4793
H	3.51163	-1.54651	1.18462
H	1.14843	-1.50957	-0.7304
H	1.1703	1.13432	-0.62553
H	1.42122	-0.30658	2.0678
O	-0.38148	-0.28007	1.21642
O	-1.85221	0.99681	0.04698
O	3.01414	0.92812	0.31935
C	-3.25506	2.58566	-1.03047
H	-2.39773	3.25391	-1.14508
H	-3.93585	2.74837	-1.86716
O	-3.98897	2.91611	0.15964
H	-3.36289	2.97819	0.8915
O	-4.76416	0.26104	0.17164
H	-4.82023	1.21021	0.37295
O	-4.31257	-2.30161	-0.66549
H	-4.91154	-1.9701	0.01849
O	-1.58506	-2.63306	0.23485
H	-2.25	-3.33378	0.22289
O	1.18107	-2.71592	0.94294
H	0.22356	-2.8392	0.81153
O	3.52367	-2.56877	-0.62359
H	3.05926	-3.35663	-0.31154
O	4.91094	-0.09668	-0.42596
H	5.21215	0.5785	-1.06769
C	1.27471	2.28784	1.17118
H	1.65306	3.14651	0.60492
H	0.19599	2.39183	1.28161
O	1.8285	2.27039	2.48608
H	2.78144	2.14603	2.3967

O	5.7645	1.81692	-2.24448
H	6.07243	2.65607	-1.88099
H	6.43155	1.55892	-2.89208

PC_{2w}

C	3.61372	1.11322	-0.93858
C	2.59459	1.32965	0.18462
C	1.45047	0.31835	0.08566
C	2.86409	-1.27748	-1.00293
C	4.08518	-0.34226	-0.97069
H	3.08031	1.19404	1.1567
H	3.14262	1.35877	-1.89434
H	2.34708	-1.11043	-1.95958
H	4.662	-0.51015	-1.88946
H	0.8859	0.4878	-0.84048
C	-1.19838	1.78771	0.28087
C	-2.71943	1.88655	0.21424
C	-3.30381	0.61071	-0.39104
C	-1.42493	-0.72202	0.46493
C	-0.78627	0.54157	1.06779
H	-2.9498	0.4794	-1.42285
H	-3.1246	1.9963	1.2291
H	-0.82965	1.72063	-0.75129
H	-1.02818	-0.91101	-0.5415
H	-1.13958	0.64721	2.09476
O	0.63956	0.44431	1.21845
O	1.96623	-1.00748	0.08388
O	-2.85438	-0.53287	0.38754
C	3.21272	-2.76037	-0.93017
H	2.29844	-3.35369	-1.01202
H	3.8694	-3.01833	-1.76203
O	3.92441	-3.10372	0.26971
H	3.30017	-3.08671	1.00549
O	4.92715	-0.52632	0.16936
H	4.89833	-1.46616	0.41534
O	4.70247	2.02503	-0.79793
H	5.27578	1.67794	-0.09988
O	2.01817	2.63696	0.09921
H	2.73829	3.27966	0.05994
O	-0.71386	2.9856	0.87518
H	0.24683	3.02268	0.71638
O	-3.11092	2.99024	-0.59415
H	-2.56535	3.73946	-0.31998
O	-4.68028	0.65198	-0.32596
H	-5.07001	0.08082	-1.02507
C	-1.19711	-1.97098	1.31154
H	-1.6525	-2.83063	0.80734
H	-0.12603	-2.15035	1.39418
O	-1.699	-1.83955	2.63995

H	-2.64793	-1.67406	2.58532
O	-4.24908	-2.86032	-0.60914
H	-3.78285	-2.13483	-0.15197
H	-4.66896	-3.38088	0.08509
O	-5.66516	-1.11554	-2.18717
H	-6.62128	-1.22145	-2.24482
H	-5.32607	-1.91039	-1.72327

PC_{3w}

C	-4.15412	0.99536	0.66899
C	-3.06362	1.14754	-0.39699
C	-1.85189	0.27156	-0.07206
C	-3.21348	-1.28071	1.1375
C	-4.50215	-0.47968	0.88395
H	-3.45229	0.83326	-1.3714
H	-3.7889	1.41844	1.60881
H	-2.79206	-0.93187	2.09189
H	-5.13598	-0.57038	1.77559
H	-1.38149	0.61921	0.85686
C	0.69363	1.90924	-0.27117
C	2.19393	2.15638	-0.1359
C	2.87162	0.99971	0.59944
C	1.13845	-0.56706	-0.14561
C	0.43388	0.55192	-0.93203
H	2.51264	0.93495	1.63599
H	2.64007	2.22087	-1.13738
H	0.26786	1.91926	0.74088
H	0.72941	-0.63754	0.87196
H	0.84748	0.56786	-1.94178
O	-0.96673	0.31671	-1.15428
O	-2.25662	-1.08315	0.08651
O	2.54009	-0.24215	-0.07086
C	-3.42926	-2.7852	1.26202
H	-2.4775	-3.27121	1.49143
H	-4.12587	-2.98426	2.07759
O	-4.01165	-3.36112	0.0817
H	-3.33652	-3.38177	-0.60761
O	-5.22965	-0.90121	-0.27161
H	-5.1121	-1.86118	-0.36688
O	-5.29961	1.76906	0.31505
H	-5.78008	1.27174	-0.36191
O	-2.60643	2.50212	-0.46108
H	-3.37687	3.07485	-0.56815
O	0.15199	2.9905	-1.02015
H	-0.81819	2.95232	-0.93598
O	2.43714	3.35616	0.59007
H	1.85827	4.03105	0.2117
O	4.23863	1.16094	0.53447
H	4.69909	0.62819	1.22215

C	1.00773	-1.9445	-0.793
H	1.47713	-2.68861	-0.14059
H	-0.05281	-2.1836	-0.86592
O	1.54683	-2.01108	-2.11074
H	2.51105	-2.06673	-2.04063
O	4.35433	-2.17248	-0.93064
H	3.84096	-1.46809	-0.48372
H	4.18253	-2.97903	-0.42906
O	5.78186	-0.36181	2.18848
H	6.39716	0.08553	2.77971
H	6.11503	-1.83037	-0.45678
O	6.94003	-1.65978	0.04279
H	7.51272	-1.1619	-0.55118
H	6.32921	-0.80984	1.50591

2. HAc-catalyzed Mechanism

RC_{HAc}

C	3.8107	0.45399	-1.17766
C	2.98353	1.03701	-0.03128
C	1.67078	0.27663	0.12266
C	2.62991	-1.71577	-0.7687
C	3.99672	-1.05171	-0.99208
H	3.53781	0.94801	0.90846
H	3.28803	0.64024	-2.11956
H	2.05184	-1.60335	-1.69701
H	4.4306	-1.47442	-1.90678
H	1.06169	0.40793	-0.7805
C	-0.59577	2.2546	0.18805
C	-2.07695	2.60971	0.18316
C	-2.89721	1.38906	-0.2285
C	-1.25366	-0.1157	0.7845
C	-0.37403	1.08674	1.15055
H	-3.9661	1.58359	-0.10971
H	-2.37822	2.87411	1.20456
H	-0.31298	1.97344	-0.83122
H	-0.96267	-0.52609	-0.187
H	-0.63819	1.41543	2.15634
O	1.01161	0.74086	1.26183
O	1.92183	-1.10663	0.31802
O	-2.63513	0.32127	0.7125
C	2.70796	-3.20168	-0.44713
H	1.6975	-3.6125	-0.37933
H	3.24482	-3.72126	-1.24112
O	3.43115	-3.45351	0.76758
H	2.89532	-3.12845	1.50195
O	4.90554	-1.21913	0.09692
H	4.71112	-2.0711	0.52222
O	5.05802	1.13702	-1.28043
H	5.62424	0.7947	-0.57441

O	2.65663	2.4051	-0.28799
H	3.47357	2.86813	-0.51374
O	0.13128	3.41024	0.58308
H	1.06723	3.24228	0.37225
O	-2.35844	3.68434	-0.69926
H	-1.69457	4.36404	-0.52376
O	-2.57954	1.00472	-1.52434
H	-3.20611	0.29429	-1.77311
C	-1.2035	-1.23026	1.81804
H	-1.83649	-2.05883	1.48229
H	-0.17787	-1.58894	1.89017
O	-1.5858	-0.79518	3.12056
H	-2.4922	-0.46867	3.07244
C	-4.79369	-1.80023	-0.96725
O	-4.40046	-1.04861	-1.84821
O	-4.41887	-1.6889	0.3051
H	-3.77494	-0.9429	0.42374
C	-5.7424	-2.93818	-1.19769
H	-5.25848	-3.87675	-0.91806
H	-6.62039	-2.81926	-0.55938
H	-6.04134	-2.97155	-2.24231

RC_{HAc+w}

C	-4.27525	0.49847	0.67396
C	-3.29371	0.84792	-0.44553
C	-1.94137	0.18937	-0.19546
C	-2.94729	-1.59641	1.02168
C	-4.36048	-1.01614	0.86033
H	-3.67641	0.48095	-1.40317
H	-3.92729	0.95768	1.60293
H	-2.53583	-1.20999	1.96512
H	-4.92027	-1.23301	1.77872
H	-1.50381	0.58909	0.72781
C	0.22009	2.26608	-0.39822
C	1.65726	2.74845	-0.24318
C	2.46841	1.72775	0.55469
C	1.07865	-0.10335	-0.27537
C	0.21626	0.8884	-1.06611
H	3.53168	1.98065	0.53599
H	2.11245	2.8137	-1.23942
H	-0.22137	2.20505	0.60182
H	0.66804	-0.25553	0.7276
H	0.63429	0.98438	-2.06897
O	-1.11706	0.41534	-1.29823
O	-2.09678	-1.21612	-0.06675
O	2.4018	0.46596	-0.14604
C	-2.90511	-3.11676	1.08625
H	-1.88007	-3.44403	1.27747
H	-3.54202	-3.46691	1.89886

O	-3.40603	-3.72274	-0.11533
H	-2.77174	-3.54533	-0.82116
O	-5.06897	-1.52622	-0.27014
H	-4.77	-2.43771	-0.42596
O	-5.55155	1.07517	0.40617
H	-5.97585	0.51884	-0.26231
O	-3.0775	2.25999	-0.50485
H	-3.94084	2.69214	-0.52933
O	-0.4818	3.23196	-1.17031
H	-1.43141	3.03702	-1.07584
O	1.71867	4.01145	0.40152
H	1.06569	4.57377	-0.03525
O	1.98499	1.6152	1.84724
H	2.63114	1.07228	2.35421
C	1.20631	-1.46845	-0.93735
H	1.81746	-2.11673	-0.30137
H	0.20765	-1.89925	-0.99939
O	1.72783	-1.41748	-2.26334
H	2.68866	-1.33844	-2.20978
O	3.92735	0.08038	2.97947
H	4.30862	-0.49204	2.28373
H	3.70482	-0.50636	3.71059
C	5.19506	-1.62755	-0.18807
O	5.11158	-1.51262	1.02362
O	4.43861	-0.92683	-1.03557
H	3.77916	-0.35799	-0.55224
C	6.14112	-2.55758	-0.88571
H	6.76389	-3.07354	-0.15935
H	5.57024	-3.2834	-1.46958
H	6.76419	-1.99374	-1.58297

$TS1_{HAc}$

C	3.66967	0.5822	-1.2734
C	2.85391	1.15245	-0.11238
C	1.59546	0.3227	0.11582
C	2.63504	-1.63773	-0.75622
C	3.95113	-0.90342	-1.0516
H	3.44729	1.12638	0.80694
H	3.10079	0.70763	-2.19831
H	2.01684	-1.5862	-1.66372
H	4.37472	-1.32876	-1.9699
H	0.94528	0.39146	-0.76529
C	-0.78301	2.15673	0.22571
C	-2.27155	2.49765	0.259
C	-3.1037	1.33216	-0.25406
C	-1.24772	-0.25082	0.93457
C	-0.45436	1.02946	1.21244
H	-4.15415	1.34301	0.04895
H	-2.57435	2.71299	1.29001

H	-0.53371	1.8569	-0.79712
H	-1.02404	-0.64302	-0.06219
H	-0.69731	1.37281	2.2187
O	0.95455	0.78528	1.26822
O	1.93445	-1.03621	0.34035
O	-2.6523	0.12221	0.98148
C	2.81081	-3.10647	-0.39697
H	1.8292	-3.57	-0.27106
H	3.33955	-3.61882	-1.20105
O	3.60154	-3.2825	0.78864
H	3.07952	-2.97568	1.54047
O	4.90759	-0.98306	0.00576
H	4.78422	-1.83423	0.45835
O	4.86935	1.33278	-1.4451
H	5.48273	1.04291	-0.7551
O	2.43638	2.48986	-0.39715
H	3.21497	2.99559	-0.66325
O	-0.08379	3.34742	0.5602
H	0.84756	3.21865	0.30201
O	-2.55379	3.6104	-0.57799
H	-1.83578	4.24241	-0.43076
O	-2.80801	0.84462	-1.40325
H	-3.54729	-0.03703	-1.68886
C	-1.01284	-1.35246	1.96141
H	-1.62687	-2.21995	1.69631
H	0.03508	-1.64434	1.91594
O	-1.27318	-0.92981	3.2957
H	-2.21188	-0.72163	3.37055
C	-4.48251	-1.84891	-1.04923
O	-4.28052	-0.97774	-1.9671
O	-4.05088	-1.75765	0.12781
H	-3.23483	-0.68347	0.64135
C	-5.27735	-3.0659	-1.4449
H	-4.60605	-3.76472	-1.95307
H	-5.69223	-3.558	-0.56718
H	-6.06832	-2.79568	-2.14432

$TS1_{HAc+w}$

C	-3.94032	0.38491	1.11731
C	-3.14782	0.9403	-0.06707
C	-1.78619	0.26131	-0.16625
C	-2.60966	-1.72238	0.86394
C	-4.01982	-1.13978	1.04234
H	-3.68947	0.74882	-0.99876
H	-3.43911	0.67564	2.04415
H	-2.04045	-1.50268	1.77851
H	-4.42651	-1.52378	1.98612
H	-1.19289	0.49281	0.72735
C	0.33906	2.36773	-0.37189

C	1.76869	2.91156	-0.34907
C	2.69734	1.96662	0.39646
C	1.1475	-0.0223	-0.81719
C	0.21427	1.11497	-1.24818
H	3.76181	2.03371	0.16354
H	2.13836	3.03489	-1.3719
H	0.05609	2.14116	0.66056
H	0.92436	-0.34679	0.20545
H	0.46474	1.38926	-2.27358
O	-1.15183	0.69249	-1.33329
O	-1.94536	-1.14499	-0.26689
O	2.47922	0.53343	-0.8573
C	-2.58264	-3.22972	0.65289
H	-1.54567	-3.57127	0.60573
H	-3.07694	-3.72556	1.48865
O	-3.29126	-3.62277	-0.53257
H	-2.77983	-3.32405	-1.29491
O	-4.91092	-1.44809	-0.03021
H	-4.6614	-2.31699	-0.38709
O	-5.23296	0.984	1.1673
H	-5.76993	0.54922	0.48982
O	-2.91429	2.34184	0.09351
H	-3.76164	2.76734	0.27681
O	-0.4823	3.41635	-0.8697
H	-1.40303	3.19625	-0.63621
O	1.81708	4.15244	0.34522
H	1.01204	4.62661	0.08979
O	2.33906	1.55187	1.5373
H	3.19242	0.93635	2.10144
C	1.07711	-1.23797	-1.73759
H	1.762	-2.0052	-1.3644
H	0.06282	-1.6319	-1.7097
O	1.36534	-0.91864	-3.09626
H	2.27843	-0.61222	-3.14656
O	4.0799	0.28724	2.59586
H	4.16601	-0.68149	2.14201
H	3.9574	0.18292	3.54712
C	4.4309	-2.1469	0.36326
O	4.33679	-1.95643	1.61355
O	4.18149	-1.28165	-0.52164
H	3.17787	-0.1845	-0.61756
C	4.854	-3.52381	-0.10548
H	5.30234	-4.09963	0.70264
H	3.96722	-4.05348	-0.46668
H	5.54867	-3.43945	-0.9422

$IM1_{HAc}$

C	3.55648	0.50762	-1.4144
C	2.80223	1.15439	-0.25148

C	1.56211	0.3406	0.103	O	3.63293	-3.20341	0.9119
C	2.56786	-1.67293	-0.6848	H	3.15508	-2.84173	1.66868
C	3.85924	-0.95938	-1.1113	O	4.88045	-0.96659	-0.11289
H	3.44467	1.19353	0.63377	H	4.78721	-1.78297	0.40611
H	2.93644	0.57038	-2.31249	O	4.74051	1.24768	-1.70251
H	1.89445	-1.68725	-1.55362	H	5.39374	1.00344	-1.03164
H	4.22731	-1.44508	-2.02372	O	2.36493	2.4682	-0.60688
H	0.86763	0.33663	-0.74666	H	3.12548	2.95753	-0.94564
C	-0.82737	2.15332	0.22089	O	-0.06957	3.33761	0.45849
C	-2.29677	2.59245	0.27714	H	0.84059	3.17688	0.14589
C	-3.22941	1.58129	-0.37772	O	-2.47128	3.79948	-0.46553
C	-1.20345	-0.24808	1.13895	H	-1.6433	4.29099	-0.34368
C	-0.44882	1.0824	1.25955	O	-2.93448	0.99694	-1.40792
H	-4.23532	1.49128	0.05467	H	-3.8272	-0.36399	-1.82388
H	-2.60722	2.74328	1.31613	C	-0.7777	-1.27475	2.18849
H	-0.6298	1.7898	-0.79242	H	-1.30767	-2.21346	1.98489
H	-1.05281	-0.67985	0.14284	H	0.29205	-1.45859	2.12574
H	-0.63971	1.4957	2.2511	O	-1.05583	-0.81925	3.51151
O	0.97618	0.88605	1.24665	H	-1.98449	-0.55362	3.52692
O	1.93292	-0.99625	0.40641	C	-4.43983	-2.05855	-1.12456
O	-2.59289	0.05448	1.33247	O	-4.31611	-1.18252	-2.11392
C	2.77295	-3.11262	-0.23445	O	-4.01255	-1.86615	0.00637
H	1.80296	-3.56719	-0.01812	H	-3.12138	-0.65458	0.90722
H	3.25614	-3.68013	-1.03015	C	-5.15883	-3.30878	-1.53809

H	-4.61081	-3.79276	-2.34959
H	-5.24805	-3.98749	-0.69359
H	-6.14965	-3.05263	-1.9193

IM1$_{HAc+w}$

C	-3.52526	0.62684	1.44024
C	-2.80606	1.30972	0.2757
C	-1.56879	0.516	-0.12816
C	-2.52879	-1.52554	0.6374
C	-3.81743	-0.83711	1.11082
H	-3.47083	1.36703	-0.59189
H	-2.88431	0.6771	2.32432
H	-1.83325	-1.54921	1.48852
H	-4.15807	-1.34723	2.02048
H	-0.85588	0.49888	0.70606
C	0.83135	2.31278	-0.25819
C	2.30342	2.74667	-0.35344
C	3.24351	1.76593	0.34412
C	1.13846	-0.0726	-1.25282
C	0.41234	1.27587	-1.31507
H	4.23267	1.62309	-0.11315
H	2.60348	2.85247	-1.40049
H	0.66516	1.92381	0.7512
H	0.95651	-0.55225	-0.28435
H	0.58308	1.71565	-2.29881
O	-1.01471	1.09742	-1.26907
O	-1.93098	-0.81761	-0.45479
O	2.53718	0.20241	-1.40359
C	-2.72661	-2.95809	0.16191
H	-1.75623	-3.39507	-0.08691
H	-3.18331	-3.54869	0.95646
O	-3.61231	-3.03596	-0.9656
H	-3.1572	-2.65148	-1.72519
O	-4.86169	-0.83486	0.13646
H	-4.77185	-1.63922	-0.40152
O	-4.71094	1.3444	1.7742
H	-5.37689	1.10862	1.11296
O	-2.36596	2.61681	0.65261
H	-3.12082	3.09654	1.0166
O	0.06649	3.50347	-0.44032
H	-0.83552	3.33505	-0.10914
O	2.49078	3.98534	0.33319
H	1.64111	4.44834	0.25185
O	2.97182	1.26795	1.42073
H	4.02367	0.11605	2.25117
C	0.69967	-1.02886	-2.36282
H	1.20011	-1.99194	-2.20728
H	-0.37553	-1.18594	-2.32286
O	1.00794	-0.50962	-3.65547

H	1.94331	-0.26836	-3.6451
O	4.53366	-0.61554	2.66491
H	3.85406	-2.02102	2.17169
H	4.53161	-0.44137	3.61303
C	3.18509	-2.83354	0.56696
O	3.37252	-2.8526	1.87714
O	3.63912	-1.94981	-0.1501
H	3.02286	-0.57424	-1.0618
C	2.35105	-3.97566	0.06299
H	2.60753	-4.90028	0.58026
H	1.30035	-3.75586	0.27469
H	2.479	-4.08945	-1.01119

IM2$_{HAc}$

C	3.79971	0.67231	-1.365
C	2.96469	1.19624	-0.19564
C	1.74569	0.31066	0.04132
C	2.86856	-1.59357	-0.85865
C	4.14857	-0.80107	-1.16046
H	3.56463	1.19556	0.7197
H	3.22205	0.78213	-2.28629
H	2.23867	-1.56173	-1.75909
H	4.58184	-1.19921	-2.08643
H	1.08266	0.35264	-0.83251
C	-0.75783	1.98833	0.23142
C	-2.23425	2.41407	0.3241
C	-3.18077	1.47109	-0.39561
C	-1.00772	-0.49891	0.92164
C	-0.33519	0.85419	1.18743
H	-2.76417	0.93429	-1.26263
H	-2.54523	2.50862	1.36979
H	-0.55755	1.6994	-0.80881
H	-0.72888	-0.86647	-0.07329
H	-0.57618	1.16365	2.20448
O	1.09854	0.74123	1.20107
O	2.15664	-1.03216	0.25051
C	3.11139	-3.05618	-0.51303
H	2.1521	-3.5638	-0.38521
H	3.65788	-3.53853	-1.32376
O	3.91569	-3.2056	0.66722
H	3.38629	-2.92106	1.42271
O	5.11779	-0.84867	-0.11256
H	5.03301	-1.70681	0.33572
O	4.96403	1.4776	-1.53355
H	5.59336	1.20662	-0.85027
O	2.48441	2.51338	-0.47429
H	3.23742	3.06553	-0.7205
O	-0.02154	3.16935	0.54027
H	0.9014	3.0455	0.24676

O	-2.40371	3.65833	-0.36052
H	-1.56046	4.12595	-0.24511
O	-4.37809	1.43724	-0.16015
C	-0.60599	-1.56951	1.92775
H	-1.18921	-2.47379	1.71627
H	0.4536	-1.7964	1.79471
O	-0.87	-1.09837	3.2521
H	-0.53274	-1.74994	3.87484
O	-2.40989	-0.23903	0.96782
H	-5.17782	0.11592	-0.81965
C	-5.07003	-1.80551	-1.0608
O	-5.6889	-0.64184	-1.22077
O	-3.99954	-1.93	-0.48075
H	-2.91209	-0.9345	0.49512
C	-5.82027	-2.9524	-1.67272
H	-5.92704	-2.78531	-2.74695
H	-5.29147	-3.88523	-1.4936
H	-6.82491	-3.00317	-1.24783

IM2$_{HAc+w}$

C	-3.98125	-0.40674	-1.36636
C	-3.21064	-1.12247	-0.25564
C	-1.905	-0.39685	0.04641
C	-2.80937	1.69126	-0.66586
C	-4.16728	1.07187	-1.02774
H	-3.80926	-1.14248	0.6604
H	-3.41555	-0.49397	-2.29761
H	-2.1841	1.67313	-1.56983
H	-4.55237	1.59576	-1.91148
H	-1.25546	-0.43248	-0.83857
C	0.46915	-2.2888	0.08074
C	1.88617	-2.87729	0.21328
C	2.97926	-2.03456	-0.42055
C	0.85799	0.12581	0.94155
C	0.12055	-1.20444	1.12108
H	2.69165	-1.45428	-1.31176
H	2.13136	-3.05304	1.26635
H	0.35556	-1.89017	-0.93588
H	0.54237	0.60455	0.00946
H	0.34241	-1.60335	2.11216
O	-1.3033	-1.00012	1.1517
O	-2.16391	0.95798	0.38181
O	2.25389	-0.18085	0.87829
C	-2.89222	3.13508	-0.19022
H	-1.88373	3.52126	-0.02287
H	-3.37852	3.74409	-0.95266
O	-3.68116	3.26736	1.0024
H	-3.18741	2.86682	1.72879
O	-5.12785	1.13156	0.02748

H	-4.95005	1.93226	0.54897
O	-5.22617	-1.06058	-1.599
H	-5.82386	-0.78488	-0.88972
O	-2.8666	-2.45083	-0.65569
H	-3.67188	-2.90429	-0.93534
O	-0.39773	-3.40813	0.25059
H	-1.29996	-3.15916	-0.02659
O	1.95604	-4.1027	-0.52255
H	1.05623	-4.46733	-0.49109
O	4.14524	-2.12796	-0.08319
H	5.25336	-0.95806	-0.76727
C	0.61203	1.09653	2.09659
H	1.07747	2.05722	1.84574
H	-0.45555	1.25257	2.23724
O	1.1362	0.59058	3.32357
H	2.05077	0.33209	3.14892
O	5.84125	-0.24119	-1.09693
H	5.36137	1.32886	-1.02598
H	6.15748	-0.52837	-1.96078
C	4.02901	2.72603	-0.81133
O	5.26619	2.32678	-1.05665
O	3.11584	1.9606	-0.52894
H	2.70105	0.54455	0.39495
C	3.85738	4.2138	-0.91976
H	4.54475	4.71281	-0.23324
H	4.11158	4.53876	-1.93118
H	2.83227	4.49174	-0.68737

$TS2_{HAc}$

C	3.88293	0.69534	-1.20906
C	2.99806	1.18403	-0.06129
C	1.75308	0.31382	0.0647
C	2.87832	-1.57143	-0.86339
C	4.18909	-0.79384	-1.05282
H	3.54834	1.12745	0.88301
H	3.35637	0.85856	-2.15293
H	2.30187	-1.48169	-1.79504
H	4.66744	-1.15951	-1.96985
H	1.14084	0.41911	-0.83994
C	-0.71674	2.04118	0.18397
C	-2.20796	2.38059	0.21883
C	-3.05606	1.25981	-0.34553
C	-1.08271	-0.42084	0.73517
C	-0.36375	0.87569	1.11776
H	-2.69703	0.8286	-1.28601
H	-2.52449	2.57252	1.25076
H	-0.45578	1.78927	-0.85188
H	-0.778	-0.76561	-0.25873
H	-0.65838	1.14597	2.13225

O	1.05269	0.70063	1.21058
O	2.11314	-1.0474	0.22989
C	3.07143	-3.0541	-0.57809
H	2.09608	-3.54441	-0.52662
H	3.64999	-3.50887	-1.38253
O	3.80804	-3.28022	0.63346
H	3.24334	-3.02681	1.37428
O	5.09328	-0.9103	0.04617
H	4.97233	-1.7895	0.44225
O	5.07056	1.48002	-1.28141
H	5.65679	1.16814	-0.5776
O	2.55359	2.52185	-0.29925
H	3.32732	3.06711	-0.49068
O	-0.03638	3.22719	0.56635
H	0.90621	3.11863	0.33823
O	-2.46608	3.51502	-0.60059
H	-1.72023	4.11677	-0.4609
O	-4.31916	1.30581	-0.15431
C	-0.86365	-1.55433	1.7324
H	-1.42612	-2.43298	1.39805
H	0.19592	-1.80507	1.74041
O	-1.22088	-1.19445	3.06215
H	-2.16674	-1.00648	3.08144
O	-2.49407	-0.09477	0.71648
H	-4.84592	0.41577	-0.69575
C	-4.89868	-1.71832	-0.98276
O	-5.39026	-0.56416	-1.23891
O	-3.86274	-1.91593	-0.29751
H	-3.06715	-0.87861	0.31479
C	-5.64788	-2.90436	-1.5338
H	-6.026	-2.68581	-2.53262
H	-5.01479	-3.78957	-1.54867
H	-6.5088	-3.09887	-0.88723

$TS2_{HAc+w}$

C	-3.908	-0.59864	-1.35737
C	-3.09083	-1.24412	-0.23691
C	-1.84193	-0.42288	0.05999
C	-2.89002	1.58654	-0.68123
C	-4.19977	0.86639	-1.03344
H	-3.68914	-1.29513	0.67805
H	-3.33656	-0.65559	-2.2876
H	-2.26535	1.60263	-1.58555
H	-4.62314	1.3516	-1.92169
H	-1.18363	-0.42836	-0.81858
C	0.59876	-2.2066	0.1125
C	2.06811	-2.61982	0.22394
C	3.0185	-1.55151	-0.26491
C	0.94328	0.18755	0.93815

C	0.21171	-1.13957	1.14503
H	2.74716	-1.02696	-1.18446
H	2.31501	-2.86292	1.26356
H	0.42439	-1.833	-0.90482
H	0.64199	0.65197	-0.00618
H	0.45097	-1.52029	2.13861
O	-1.20932	-0.96295	1.18273
O	-2.19256	0.91427	0.37505
C	-3.07615	3.02587	-0.22146
H	-2.09775	3.48606	-0.06287
H	-3.60783	3.58917	-0.98866
O	-3.86832	3.11413	0.97262
H	-3.34453	2.75861	1.70142
O	-5.1604	0.86669	0.02343
H	-5.04011	1.68238	0.53791
O	-5.10212	-1.34314	-1.58413
H	-5.71955	-1.10535	-0.878
O	-2.65301	-2.55056	-0.61871
H	-3.42256	-3.05407	-0.91339
O	-0.1456	-3.3998	0.31258
H	-1.0677	-3.23196	0.03907
O	2.32236	-3.73828	-0.62171
H	1.51032	-4.26791	-0.60252
O	4.23861	-1.65075	0.04254
C	0.69884	1.18462	2.06855
H	1.23633	2.10953	1.83874
H	-0.36713	1.40018	2.12071
O	1.08764	0.67032	3.33988
H	2.03292	0.48004	3.30566
O	2.3534	-0.12068	0.88839
H	4.91712	-0.9325	-0.57308
O	5.61915	-0.12576	-1.19829
H	5.1172	0.79011	-1.40227
H	5.94493	-0.49193	-2.0292
C	3.7795	2.61457	-0.85965
O	4.51455	2.02915	-1.71106
O	3.35318	2.09248	0.20743
H	2.85271	0.71762	0.57558
C	3.41033	4.06046	-1.12769
H	3.61138	4.33637	-2.16179
H	2.36021	4.23202	-0.88686
H	4.0077	4.6998	-0.47095

PC_{HAc}

C	3.9761	0.56236	-1.11935
C	3.09054	1.07066	0.0189
C	1.79156	0.27471	0.08255
C	2.83233	-1.6498	-0.86337
C	4.19071	-0.94589	-0.99824

H	3.60863	0.94973	0.97551	O	5.20908	1.27763	-1.1401
H	3.48554	0.7821	-2.07113	H	5.75633	0.91478	-0.4294
H	2.28891	-1.50372	-1.80781	O	2.74027	2.44142	-0.18722
H	4.67025	-1.31403	-1.91372	H	3.55274	2.93386	-0.36082
H	1.21688	0.43599	-0.83817	O	0.15873	3.33461	0.59618
C	-0.53824	2.18006	0.15267	H	1.10525	3.18658	0.41705
C	-2.0213	2.52386	0.10028	O	-2.25569	3.57893	-0.82235
C	-2.82051	1.30554	-0.34665	H	-1.57786	4.24643	-0.65192
C	-1.15162	-0.21935	0.60958	O	-4.16928	1.56959	-0.2596
C	-0.3137	0.98009	1.07091	C	-1.08227	-1.39858	1.56979
H	-2.52559	1.00218	-1.36062	H	-1.6885	-2.22038	1.17436
H	-2.36656	2.80708	1.10299	H	-0.04806	-1.73333	1.63166
H	-0.22225	1.9362	-0.8697	O	-1.49013	-1.05587	2.89156
H	-0.83121	-0.56005	-0.38305	H	-2.40429	-0.75021	2.85378
H	-0.62447	1.24844	2.08094	O	-2.53537	0.19174	0.54665
O	1.07676	0.67014	1.21474	H	-4.65122	0.85132	-0.72186
O	2.06732	-1.11018	0.22195	C	-5.09671	-1.7536	-0.87871
C	2.93313	-3.14783	-0.61186	O	-5.31127	-0.65642	-1.37569
H	1.93094	-3.58362	-0.60489	O	-4.1375	-1.96662	0.01879
H	3.51274	-3.61499	-1.40842	H	-3.62378	-1.13783	0.1977
O	3.61457	-3.44398	0.61687	C	-5.8752	-2.99112	-1.20811
H	3.0423	-3.17031	1.34464	H	-5.19867	-3.75917	-1.58892
O	5.05878	-1.14607	0.11787	H	-6.33775	-3.38287	-0.29945
H	4.87039	-2.02335	0.49125	H	-6.63978	-2.76684	-1.94753

PC_{HAc+w}

C	-4.41001	0.62808	0.59879
C	-3.37295	0.8895	-0.49462
C	-2.04319	0.23497	-0.13792
C	-3.12478	-1.44993	1.15339
C	-4.52161	-0.86917	0.88623
H	-3.71714	0.46204	-1.44187
H	-4.10109	1.14813	1.50935
H	-2.74941	-1.00113	2.08437
H	-5.12649	-1.01631	1.78962
H	-1.64256	0.69304	0.77531
C	0.18931	2.2412	-0.38007
C	1.62596	2.68329	-0.15152
C	2.36745	1.64194	0.68785
C	0.96803	-0.16606	-0.08627
C	0.17097	0.8156	-0.9547
H	1.8978	1.54245	1.67633
H	2.14099	2.76825	-1.11695
H	-0.3138	2.25693	0.59547
H	0.52773	-0.2462	0.91608
H	0.63129	0.83751	-1.94284
O	-1.16911	0.38022	-1.21536
O	-2.22272	-1.15634	0.07986
O	2.3047	0.35573	0.04071
C	-3.10386	-2.9621	1.329
H	-2.09077	-3.28377	1.58288
H	-3.7749	-3.24668	2.1398
O	-3.56607	-3.65023	0.15632
H	-2.89834	-3.54177	-0.53236
O	-5.18162	-1.45162	-0.23854
H	-4.8893	-2.37566	-0.31181
O	-5.66581	1.19416	0.23113
H	-6.06422	0.59524	-0.41607
O	-3.12888	2.29	-0.64018
H	-3.98063	2.73134	-0.75094
O	-0.4572	3.14549	-1.26084
H	-1.40901	2.94556	-1.22118
O	1.62191	3.93322	0.52635
H	2.54257	4.15739	0.71198
O	3.6916	2.01804	0.78614
H	4.1084	1.52	1.52854
C	1.04508	-1.57159	-0.66985
H	1.65597	-2.19354	-0.00728
H	0.03563	-1.97979	-0.68643
O	1.53747	-1.6116	-2.0061
H	2.49955	-1.5235	-1.97869
O	4.79615	0.40617	2.6439
H	4.89209	-0.40907	2.1115

H	4.26389	0.16558	3.41035
C	5.06868	-1.8471	-0.29747
O	5.18012	-1.72261	0.9101
O	4.26853	-1.07137	-1.03657
H	3.72637	-0.45632	-0.47884
C	5.79035	-2.87539	-1.11386
H	6.30126	-2.39525	-1.95039
H	6.50302	-3.41304	-0.49366
H	5.06203	-3.5751	-1.53173

1. TFA-catalyzed Mechanism

RC_{TFA}

C	4.46107	-0.19864	-1.26698
C	3.81253	0.58938	-0.12806
C	2.37817	0.12305	0.09489
C	2.87424	-2.05968	-0.72445
C	4.33917	-1.7017	-1.01677
H	4.36937	0.42731	0.80029
H	3.95528	0.05473	-2.20234
H	2.29771	-1.86995	-1.64102
H	4.64269	-2.24117	-1.92262
H	1.77896	0.34032	-0.79811
C	0.56295	2.51893	0.11389
C	-0.81383	3.17057	0.12832
C	-1.88043	2.12821	-0.19634
C	-0.53752	0.36271	0.86025
C	0.57883	1.379	1.13348
H	-2.88146	2.54421	-0.06425
H	-1.01872	3.5408	1.14051
H	0.74371	2.13619	-0.89544
H	-0.37765	-0.14479	-0.09514
H	0.42437	1.80304	2.12619
O	1.86693	0.76143	1.22661
O	2.34605	-1.27223	0.35035
O	-1.80647	1.07402	0.79871
C	2.65704	-3.51503	-0.33411
H	1.58727	-3.7027	-0.21316
H	3.0402	-4.16652	-1.11985
O	3.36333	-3.86403	0.86648
H	2.93589	-3.40932	1.60299
O	5.23392	-2.00986	0.05292
H	4.88649	-2.78829	0.51978
O	5.81802	0.20542	-1.43391
H	6.32591	-0.21956	-0.72838
O	3.76318	1.98359	-0.44146
H	4.64805	2.25902	-0.71319
O	1.52262	3.51866	0.42537
H	2.39746	3.15319	0.20142
O	-0.90452	4.23219	-0.80703

H	-0.11064	4.77026	-0.68943
O	-1.68873	1.62395	-1.47556
H	-2.47074	1.09042	-1.70101
C	-0.66912	-0.68627	1.95376
H	-1.483	-1.37391	1.69943
H	0.25843	-1.25557	1.99061
O	-0.86236	-0.12315	3.24796
H	-1.69556	0.36225	3.24894
C	-4.42799	-0.52219	-0.5102
O	-4.03801	0.02145	-1.51721
O	-3.94134	-0.43243	0.69819
H	-3.11785	0.15467	0.72733
C	-5.65146	-1.47663	-0.53854
F	-6.20356	-1.51075	-1.7538
F	-5.27542	-2.72773	-0.21113
F	-6.58982	-1.08229	0.3405

RC_{TFA+w}

C	4.99817	0.12017	-0.54548
C	4.02051	0.52754	0.55769
C	2.6094	0.057	0.22163
C	3.44075	-1.76857	-1.06627
C	4.90572	-1.38106	-0.81548
H	4.31508	0.06443	1.50472
H	4.74661	0.66671	-1.45826
H	3.1247	-1.27915	-1.99864
H	5.47595	-1.61783	-1.7224
H	2.26167	0.56143	-0.68853
C	0.72134	2.37743	0.48291
C	-0.63515	3.04861	0.30283
C	-1.52324	2.19236	-0.599
C	-0.42136	0.14258	0.18632
C	0.52341	0.97431	1.06283
H	-2.54582	2.57708	-0.61646
H	-1.12951	3.10989	1.28035
H	1.19731	2.31921	-0.50118
H	0.00807	-0.01256	-0.80749
H	0.07982	1.06593	2.05486
O	1.77406	0.32007	1.30871
O	2.59523	-1.34667	0.01098
O	-1.6542	0.89049	0.03321
C	3.2147	-3.26508	-1.22911
H	2.16601	-3.44986	-1.47479
H	3.8364	-3.64226	-2.04151
O	3.58869	-4.0001	-0.05368
H	2.94816	-3.7953	0.63887
O	5.49212	-2.03512	0.31041
H	5.08147	-2.91181	0.39516
O	6.32249	0.52051	-0.20122

H	6.64801	-0.11662	0.45021
O	3.97572	1.95023	0.69274
H	4.8836	2.27015	0.77137
O	1.50116	3.19851	1.34173
H	2.42343	2.89411	1.26652
O	-0.50594	4.34503	-0.25853
H	0.19383	4.78969	0.23764
O	-0.982	2.08371	-1.86403
H	-1.66585	1.69466	-2.45603
C	-0.75087	-1.22328	0.77192
H	-1.43409	-1.74895	0.09782
H	0.17849	-1.78967	0.81961
O	-1.27695	-1.16872	2.09628
H	-2.22039	-0.97586	2.05185
O	-3.01121	0.98082	-3.30208
H	-3.55547	0.45548	-2.68919
H	-2.77979	0.38564	-4.024
C	-4.69913	-0.57411	-0.23095
O	-4.62891	-0.41902	-1.42594
O	-3.86601	-0.17369	0.69206
H	-3.04058	0.29042	0.31803
C	-5.89232	-1.33465	0.40842
F	-6.54853	-0.5457	1.27888
F	-5.4563	-2.4182	1.07822
F	-6.75768	-1.73977	-0.52413

$TS1_{TFA}$

C	4.19248	-0.22507	-1.55375
C	3.65153	0.66621	-0.43453
C	2.28878	0.17199	0.03782
C	2.7921	-2.06756	-0.60197
C	4.18759	-1.69024	-1.12021
H	4.33339	0.64356	0.42127
H	3.5574	-0.10757	-2.43563
H	2.09438	-1.99933	-1.44862
H	4.40665	-2.32218	-1.98986
H	1.56092	0.2612	-0.7788
C	0.35337	2.46721	0.08452
C	-0.99743	3.18134	0.20416
C	-2.15205	2.25539	-0.12019
C	-0.47235	0.32074	1.22586
C	0.57375	1.43999	1.20484
H	-3.11379	2.45819	0.35183
H	-1.12942	3.55601	1.22437
H	0.39045	1.98068	-0.89544
H	-0.46458	-0.23759	0.28362
H	0.53603	1.96473	2.16025
O	1.90646	0.92024	1.15518
O	2.36863	-1.18414	0.44449

O	-1.7531	0.9802	1.3766
C	2.69902	-3.47817	-0.03783
H	1.66477	-3.68823	0.24602
H	3.00591	-4.19651	-0.79855
O	3.57363	-3.67258	1.08413
H	3.2204	-3.16636	1.8263
O	5.22136	-1.82904	-0.14517
H	4.98585	-2.5707	0.43687
O	5.49186	0.21195	-1.94384
H	6.10942	-0.10774	-1.27096
O	3.47831	2.00822	-0.89676
H	4.30896	2.29929	-1.29426
O	1.33428	3.49281	0.1462
H	2.17361	3.11919	-0.18352
O	-1.07871	4.24899	-0.73026
H	-0.19252	4.64128	-0.75252
O	-2.11175	1.57618	-1.18138
H	-3.04459	0.91997	-1.31876
C	-0.29038	-0.66195	2.37894
H	-1.07966	-1.42037	2.32033
H	0.67223	-1.15751	2.26822
O	-0.29098	-0.02127	3.64986
H	-1.14876	0.40244	3.77342
C	-4.27693	-0.6052	-0.43457
O	-4.03896	0.14169	-1.43145
O	-3.73148	-0.63717	0.67008
H	-2.48129	0.3259	1.18755
C	-5.42484	-1.62106	-0.70484
F	-6.52329	-1.00276	-1.18198
F	-5.03646	-2.52957	-1.62728
F	-5.78136	-2.29086	0.39992

$TS1_{TFA+w}$

C	4.39859	-0.54273	-1.17128
C	3.83312	0.23766	0.01633
C	2.33464	-0.00692	0.15528
C	2.50934	-2.15649	-0.85596
C	4.02417	-2.02142	-1.06998
H	4.31629	-0.09187	0.9415
H	3.98493	-0.12797	-2.09409
H	2.01083	-1.78729	-1.7637
H	4.27706	-2.51997	-2.01402
H	1.81415	0.38037	-0.72973
C	0.91349	2.62206	0.36248
C	-0.28223	3.5797	0.3668
C	-1.46284	2.99474	-0.3868
C	-0.5329	0.56451	0.89567
C	0.69621	1.40133	1.26716
H	-2.46309	3.32931	-0.1074

H	-0.59046	3.7951	1.39426
H	1.08072	2.30663	-0.67193
H	-0.44599	0.17489	-0.12526
H	0.56962	1.75534	2.29084
O	1.88756	0.60789	1.32705
O	2.07279	-1.39568	0.27728
O	-1.65311	1.47141	0.96562
C	2.04077	-3.58523	-0.61834
H	0.95038	-3.60293	-0.54828
H	2.34856	-4.21513	-1.45325
O	2.62568	-4.15683	0.5619
H	2.2415	-3.71134	1.32732
O	4.80746	-2.56777	-0.00818
H	4.31908	-3.31841	0.36948
O	5.80916	-0.35471	-1.2554
H	6.20836	-0.9211	-0.58001
O	4.01812	1.6436	-0.16808
H	4.94918	1.80013	-0.37119
O	2.02694	3.38397	0.81177
H	2.83382	2.89646	0.56074
O	0.04893	4.78549	-0.31262
H	0.97698	4.95923	-0.09253
O	-1.2701	2.47581	-1.51121
H	-2.27287	2.15408	-2.09347
C	-0.76616	-0.60958	1.84381
H	-1.658	-1.15349	1.51716
H	0.09077	-1.27807	1.78797
O	-0.89069	-0.20097	3.20375
H	-1.66406	0.37073	3.27666
O	-3.29276	1.81918	-2.62428
H	-3.65788	0.93659	-2.22985
H	-3.18549	1.71678	-3.57873
C	-4.25936	-0.57938	-0.46963
O	-4.22356	-0.3338	-1.69364
O	-3.79544	0.05437	0.49429
H	-2.48732	0.98422	0.70859
C	-4.98836	-1.89994	-0.06713
F	-5.94041	-1.6684	0.86343
F	-4.10672	-2.77564	0.47301
F	-5.58239	-2.52017	-1.10062

$IM1_{TFA}$

C	4.02947	-0.39583	-1.64506
C	3.58715	0.57597	-0.55007
C	2.23923	0.15734	0.02739
C	2.64592	-2.13502	-0.49407
C	4.01207	-1.83359	-1.12737
H	4.31799	0.57662	0.26472
H	3.34264	-0.30797	-2.49075

H	1.89467	-2.10547	-1.2961
H	4.1507	-2.52023	-1.97182
H	1.46979	0.21218	-0.75331
C	0.38153	2.5138	0.03675
C	-0.92357	3.31588	0.13789
C	-2.14124	2.4926	-0.25439
C	-0.44468	0.43788	1.36327
C	0.61338	1.53738	1.20396
H	-3.07964	2.71529	0.26851
H	-1.06042	3.68865	1.15795
H	0.36668	1.97458	-0.91551
H	-0.51906	-0.15503	0.44465
H	0.64356	2.11916	2.12641
O	1.93702	0.98553	1.11075
O	2.3137	-1.17373	0.51503
O	-1.69061	1.11415	1.60683
C	2.55865	-3.50056	0.17343
H	1.53926	-3.66567	0.53094
H	2.80694	-4.27848	-0.54887
O	3.49396	-3.63374	1.25481
H	3.19889	-3.05951	1.97256
O	5.10877	-1.9533	-0.22046
H	4.88368	-2.63472	0.43496
O	5.3128	-0.02315	-2.14144
H	5.963	-0.3234	-1.49073
O	3.43354	1.89422	-1.0815
H	4.24457	2.12586	-1.55192
O	1.4201	3.48908	0.01605
H	2.22312	3.06236	-0.33831
O	-0.89723	4.40509	-0.78323
H	0.032	4.68373	-0.81605
O	-2.11945	1.72148	-1.20494
H	-3.3026	0.73846	-1.39155
C	-0.15901	-0.50304	2.53288
H	-0.92914	-1.28415	2.54299
H	0.81173	-0.97531	2.40273
O	-0.13085	0.19122	3.77796
H	-0.96363	0.67377	3.85559
C	-4.26383	-0.6501	-0.44195
O	-4.03796	0.04212	-1.5207
O	-3.74578	-0.548	0.64757
H	-2.41896	0.50293	1.38905
C	-5.35311	-1.72654	-0.69915
F	-6.48043	-1.16761	-1.17502
F	-4.91973	-2.62293	-1.60688
F	-5.65446	-2.38372	0.42402

$IM1_{TFA+w}$

C	3.68922	0.02931	-1.48113

C	3.1922	0.97074	-0.38275	H	2.39229	-3.87946	-0.58557
C	1.81887	0.53519	0.11538	O	2.99745	-3.31061	1.27257
C	2.24323	-1.73947	-0.45735	H	2.66756	-2.76912	2.00043
C	3.64195	-1.42255	-1.0064	O	4.68554	-1.56896	-0.04254
H	3.88327	0.95206	0.46575	H	4.42918	-2.27805	0.5706
H	3.04713	0.14341	-2.35848	O	4.99768	0.41031	-1.89962
H	1.53555	-1.67762	-1.29633	H	5.61245	0.08798	-1.22548
H	3.82745	-2.08507	-1.86098	O	3.05539	2.3033	-0.88307
H	1.09112	0.61659	-0.70248	H	3.89244	2.56091	-1.28983
C	-0.08006	2.86471	0.11555	O	0.95758	3.84141	0.17643
C	-1.39776	3.65496	0.20786	H	1.7768	3.43169	-0.15982
C	-2.57492	2.89456	-0.39795	O	-1.30247	4.85539	-0.55876
C	-0.8924	0.69685	1.309	H	-0.36087	5.09265	-0.53776
C	0.119	1.84614	1.25235	O	-2.47966	2.29465	-1.45335
H	-3.54704	3.01265	0.10041	H	-3.77228	1.33103	-2.05197
H	-1.62438	3.89691	1.25104	C	-0.68002	-0.21404	2.51843
H	-0.05522	2.36798	-0.85934	H	-1.38217	-1.05206	2.44688
H	-0.81611	0.09292	0.39916	H	0.33369	-0.60790	2.51570
H	0.08613	2.39026	2.19738	O	-0.85987	0.49004	3.74643
O	1.46222	1.33296	1.20378	H	-1.72596	0.91533	3.70521
O	1.86314	-0.81088	0.56494	O	-4.43596	0.64032	-2.2928
O	-2.19946	1.28631	1.39168	H	-3.87038	-0.71256	-1.98355
C	2.11527	-3.12764	0.15394	H	-4.67354	0.78874	-3.21573
H	1.07952	-3.29757	0.45531	C	-3.18672	-1.78301	-0.51462

O	-3.43589	-1.62964	-1.77864
O	-3.44788	-1.03564	0.40236
H	-2.83839	0.60364	1.12684
C	-2.43537	-3.11851	-0.2562
F	-2.24258	-3.3187	1.05135
F	-1.22651	-3.09515	-0.85605
F	-3.11821	-4.16843	-0.74635

IM2$_{TFA}$

C	4.4565	0.00008	-1.58209
C	3.83025	0.81609	-0.45032
C	2.5049	0.20175	-0.01478
C	3.20016	-1.97447	-0.69612
C	4.56579	-1.47197	-1.18687
H	4.49997	0.82942	0.41508
H	3.82424	0.08899	-2.46924
H	2.50943	-1.94568	-1.55078
H	4.84438	-2.05982	-2.07032
H	1.78995	0.24903	-0.84662
C	0.31528	2.28765	0.09624
C	-1.05269	2.97572	0.25802
C	-2.21378	2.1384	-0.23824
C	-0.23144	-0.02646	1.1322
C	0.64537	1.23018	1.16971
H	-2.00336	1.45074	-1.07019
H	-1.22644	3.25070	1.30364
H	0.35041	1.83569	-0.90363
H	-0.08757	-0.56300	0.18853
H	0.53956	1.69985	2.1487
O	2.04007	0.89301	1.10618
O	2.69234	-1.15307	0.36251
C	3.2179	-3.39946	-0.16104
H	2.20087	-3.70200	0.10058
H	3.59742	-4.07422	-0.92874
O	4.08738	-3.54030	0.97299
H	3.68265	-3.07440	1.71533
O	5.59826	-1.55429	-0.20390
H	5.41147	-2.32097	0.36345
O	5.72064	0.55095	-1.94266
H	6.35374	0.26480	-1.26913
O	3.55084	2.14899	-0.88477
H	4.35908	2.52511	-1.25581
O	1.26001	3.35115	0.16615
H	2.12072	3.02880	-0.16384
O	-1.09653	4.13440	-0.57712
H	-0.17977	4.45311	-0.61547
O	-3.36356	2.34013	0.12821
C	0.05244	-0.98316	2.28933
H	-0.56052	-1.88291	2.15512

H	1.10066	-1.27418	2.2805
O	-0.21127	-0.37870	3.55322
H	-1.11675	-0.04397	3.52686
O	-1.58156	0.44516	1.22802
H	-4.41266	1.30193	-0.32156
C	-4.73253	-0.6148	-0.37468
O	-5.11516	0.60939	-0.59523
O	-3.68798	-1.01283	0.09041
H	-2.21011	-0.21714	0.88704
C	-5.83671	-1.61791	-0.80721
F	-5.4569	-2.87872	-0.58186
F	-6.97645	-1.39445	-0.1265
F	-6.10708	-1.48924	-2.12015

IM2$_{TFA+w}$

C	-3.74232	-0.31354	-1.53283
C	-3.12511	-1.33023	-0.57004
C	-1.85598	-0.76618	0.05563
C	-2.61761	1.47176	-0.18222
C	-3.93397	1.03828	-0.84374
H	-3.83098	-1.56055	0.23398
H	-3.07118	-0.18966	-2.38685
H	-1.88282	1.64302	-0.98204
H	-4.19710	1.78963	-1.59865
H	-1.11309	-0.58919	-0.73295
C	0.48701	-2.61959	-0.21278
C	1.92735	-3.16638	-0.18776
C	2.9621	-2.11059	-0.54121
C	0.76512	-0.59542	1.39729
C	0.03175	-1.89858	1.07086
H	2.60434	-1.29154	-1.18654
H	2.16739	-3.60794	0.78464
H	0.40354	-1.94465	-1.07409
H	0.55248	0.1523	0.62751
H	0.14803	-2.59189	1.90504
O	-1.3876	-1.67012	1.00994
O	-2.13158	0.46203	0.71038
O	2.16461	-0.90166	1.40302
C	-2.71968	2.75353	0.63177
H	-1.72921	3.02545	1.00503
H	-3.08894	3.56073	-0.00141
O	-3.64812	2.63053	1.72027
H	-3.25954	2.03628	2.3743
O	-5.01351	0.87669	0.07712
H	-4.88853	1.51388	0.80015
O	-4.96486	-0.8178	-2.06429
H	-5.6373	-0.70367	-1.37794
O	-2.74994	-2.52363	-1.2621
H	-3.51857	-2.85095	-1.74599

O	-0.34426	-3.75744	-0.43001
H	-1.22861	-3.44923	-0.70394
O	2.07859	-4.1368	-1.22743
H	1.19363	-4.51891	-1.34883
O	4.14497	-2.22559	-0.28138
H	5.06296	-0.79357	-0.70125
C	0.36549	-0.01978	2.75524
H	0.86011	0.95103	2.87850
H	-0.71105	0.13218	2.79390
O	0.70986	-0.89977	3.82371
H	1.64722	-1.11132	3.72658
O	5.44842	0.09401	-0.89520
H	4.42905	1.19242	-1.13804
H	6.08537	-0.03051	-1.60870
C	2.96010	2.18281	-0.33953
O	3.74396	1.93525	-1.34410
O	2.97001	1.68478	0.76495
H	2.65225	-0.06657	1.29946
C	1.88627	3.24167	-0.71398
F	1.17538	3.60508	0.35828
F	2.44125	4.34451	-1.24542
F	1.03261	2.72736	-1.62410

$TS2_{TFA}$

C	4.4423	0.01602	-1.53338
C	3.79667	0.82368	-0.40662
C	2.46428	0.20489	-0.00081
C	3.17109	-1.96609	-0.68347
C	4.54508	-1.45853	-1.14541
H	4.45077	0.82961	0.47068
H	3.8252	0.11057	-2.43054
H	2.49641	-1.93294	-1.5506
H	4.84006	-2.04058	-2.02739
H	1.76464	0.26106	-0.8449
C	0.29876	2.31078	0.06999
C	-1.0866	2.95456	0.21255
C	-2.2007	2.01509	-0.17485
C	-0.31856	0.02832	1.06699
C	0.59627	1.25371	1.14743
H	-2.03832	1.36496	-1.03748
H	-1.24691	3.29215	1.24219
H	0.35982	1.86068	-0.92928
H	-0.16659	-0.51004	0.12596
H	0.47105	1.71811	2.12629
O	1.97893	0.88531	1.11983
O	2.64093	-1.15163	0.37055
C	3.18100	-3.39452	-0.15747
H	2.16015	-3.69913	0.08611
H	3.57242	-4.06349	-0.92426

O	4.0331	-3.54372	0.98851
H	3.61498	-3.08827	1.72984
O	5.55931	-1.54585	-0.14427
H	5.36477	-2.31815	0.41279
O	5.71193	0.56966	-1.86861
H	6.33367	0.27995	-1.18607
O	3.52494	2.16045	-0.83464
H	4.33801	2.53521	-1.19662
O	1.21603	3.39051	0.16031
H	2.08847	3.07863	-0.14911
O	-1.20738	4.04362	-0.69678
H	-0.32103	4.43453	-0.75061
O	-3.37808	2.27053	0.18518
C	-0.12616	-0.9456	2.22645
H	-0.80613	-1.79458	2.08996
H	0.89695	-1.31715	2.20640
O	-0.3276	-0.32997	3.49383
H	-1.23442	-0.00192	3.52633
O	-1.66352	0.55108	1.11156
H	-4.11807	1.49677	-0.21735
C	-4.59148	-0.60816	-0.34913
O	-4.91219	0.58692	-0.62743
O	-3.58717	-1.03997	0.21932
H	-2.33098	-0.13501	0.83692
C	-5.66004	-1.63858	-0.81824
F	-6.83893	-1.41714	-0.19792
F	-5.87531	-1.53669	-2.14668
F	-5.29686	-2.90282	-0.5612

$TS2_{TFA+w}$

C	4.18752	-0.2119	-1.50145
C	3.65336	0.77331	-0.46056
C	2.27789	0.33896	0.03188
C	2.74648	-1.95299	-0.42449
C	4.15173	-1.64019	-0.95882
H	4.32787	0.81105	0.40034
H	3.56198	-0.15002	-2.39587
H	2.05633	-1.94377	-1.28012
H	4.36389	-2.33931	-1.77731
H	1.565	0.37731	-0.80215
C	0.31996	2.63376	-0.08952
C	-0.9894	3.42598	0.01592
C	-2.20837	2.60272	-0.32056
C	-0.46885	0.5295	1.14667
C	0.54504	1.67268	1.0885
H	-2.12317	1.87009	-1.12716
H	-1.10631	3.8445	1.02134
H	0.30732	2.07807	-1.03617
H	-0.34912	-0.13207	0.28285

H	0.48677	2.24615	2.01436
O	1.89096	1.17916	1.07883
O	2.32857	-0.98239	0.54360
C	2.6263	-3.3111	0.25233
H	1.58597	-3.48221	0.53994
H	2.93111	-4.09411	-0.44236
O	3.48547	-3.42393	1.39713
H	3.13167	-2.85274	2.09028
O	5.17739	-1.7255	0.03109
H	4.91768	-2.40707	0.6733
O	5.49804	0.17006	-1.91134
H	6.10390	-0.10863	-1.21019
O	3.50084	2.07599	-1.03014
H	4.33954	2.33152	-1.43485
O	1.34315	3.61895	-0.13290
H	2.17149	3.19037	-0.42300
O	-1.00331	4.46428	-0.96139
H	-0.0752	4.72781	-1.06852
O	-3.33754	3.01147	0.02426
C	-0.35176	-0.30739	2.41884
H	-1.08051	-1.12319	2.36641
H	0.64777	-0.73528	2.47416
O	-0.54386	0.47218	3.59657
H	-1.41903	0.87533	3.5419
O	-1.77487	1.13701	1.1036
H	-4.23954	2.39492	-0.45345
O	-5.15573	1.74097	-0.89832
H	-4.92042	0.74296	-1.00296
H	-5.46947	2.07614	-1.74802
C	-3.89612	-1.34807	-0.38327
O	-4.61258	-0.71561	-1.18725
O	-3.25507	-0.95462	0.60677
H	-2.43951	0.41643	0.91665
C	-3.77477	-2.88278	-0.64415
F	-4.22782	-3.5884	0.41759
F	-4.46049	-3.30016	-1.722
F	-2.48077	-3.23293	-0.83242

PC_{TFA}

C	4.59808	-0.11503	-1.25164
C	3.89283	0.6478	-0.12927
C	2.46645	0.13992	0.04973
C	3.04825	-2.02249	-0.76973
C	4.51102	-1.62209	-1.01231
H	4.42664	0.49797	0.81445
H	4.11464	0.12883	-2.20122
H	2.49577	-1.84213	-1.70284
H	4.85883	-2.14797	-1.91022
H	1.88683	0.34968	-0.85803

C	0.57109	2.47956	0.05645
C	-0.81231	3.1164	0.04699
C	-1.86723	2.06659	-0.27688
C	-0.47815	0.29072	0.72977
C	0.60236	1.32846	1.05934
H	-1.70744	1.64972	-1.27892
H	-1.03365	3.52432	1.04173
H	0.76918	2.10358	-0.95553
H	-0.28731	-0.17719	-0.24326
H	0.40631	1.72532	2.05562
O	1.90763	0.75379	1.17328
O	2.4647	-1.25748	0.29279
C	2.86003	-3.48593	-0.39472
H	1.79272	-3.70548	-0.31194
H	3.28916	-4.12105	-1.17001
O	3.53423	-3.82123	0.82791
H	3.06659	-3.38578	1.55154
O	5.37846	-1.91072	0.08482
H	5.03678	-2.69956	0.53827
O	5.94738	0.32826	-1.37412
H	6.44526	-0.0864	-0.65545
O	3.81079	2.04133	-0.43861
H	4.69549	2.34756	-0.67560
O	1.51048	3.49428	0.37398
H	2.39617	3.14317	0.16767
O	-0.88679	4.13696	-0.93748
H	-0.07812	4.65934	-0.85117
O	-3.12486	2.61256	-0.13902
C	-0.58637	-0.8057	1.78102
H	-1.37206	-1.51124	1.49146
H	0.3603	-1.34285	1.8082
O	-0.81403	-0.29641	3.09144
H	-1.66389	0.15937	3.09974
O	-1.7607	0.96801	0.68172
H	-3.76814	2.03332	-0.58522
C	-4.63011	-0.49233	-0.43465
O	-4.75029	0.52144	-1.08294
O	-3.70614	-0.78809	0.43866
H	-3.00791	-0.06266	0.52190
C	-5.63867	-1.66238	-0.58192
F	-6.62068	-1.34302	-1.42801
F	-5.01712	-2.76039	-1.05167
F	-6.18806	-1.97243	0.60591

PC_{TFA+w}

C	-5.15436	0.28349	0.34625
C	-4.06712	0.55774	-0.69363
C	-2.70464	0.11526	-0.17247
C	-3.68631	-1.54831	1.22167

C	-5.11389	-1.17823	0.79197	O	-5.60551	-1.95114	-0.30378
H	-4.27783	-0.00543	-1.60845	H	-5.20488	-2.83502	-0.2512
H	-4.98491	0.92987	1.21121	O	-6.43248	0.64706	-0.17017
H	-3.44784	-0.96059	2.11964	H	-6.70412	-0.06177	-0.77021
H	-5.77062	-1.3056	1.66152	O	-3.97581	1.95502	-0.97856
H	-2.43655	0.71192	0.70847	H	-4.85984	2.273	-1.20179
C	-0.69807	2.34066	-0.46881	O	-1.37723	3.0727	-1.47464
C	0.66034	2.97071	-0.20326	H	-2.29967	2.76125	-1.47853
C	1.44774	2.11756	0.79173	O	0.46789	4.27301	0.33154
C	0.3217	0.07586	0.11086	H	1.342	4.63045	0.53271
C	-0.51267	0.87597	-0.89698	O	2.71036	2.65058	0.93143
H	0.9191	2.05611	1.75202	H	3.11183	2.31098	1.76509
H	1.23313	3.01566	-1.13839	C	0.60206	-1.35406	-0.33432
H	-1.2661	2.39008	0.46918	H	1.25771	-1.83241	0.40025
H	-0.17768	0.02789	1.08645	H	-0.34773	-1.88662	-0.34105
H	0.01496	0.86387	-1.85106	O	1.14217	-1.45211	-1.64970
O	-1.76848	0.25758	-1.19754	H	2.08373	-1.24498	-1.62162
O	-2.73668	-1.25706	0.18858	O	3.83802	1.44814	3.07376
O	1.57747	0.76879	0.28105	H	4.09895	0.60842	2.65800
C	-3.50373	-3.01927	1.56869	H	3.28204	1.21403	3.82553
H	-2.48533	-3.1834	1.92974	C	4.64776	-0.75717	0.18019
H	-4.20381	-3.29981	2.35597	O	4.70608	-0.66309	1.38091
O	-3.78096	-3.87714	0.45103	O	3.75186	-0.26033	-0.63535
H	-3.07748	-3.75295	-0.1983	H	2.99902	0.22562	-0.16648

C	5.72245	-1.54478	-0.61741
F	5.15603	-2.54436	-1.31856
F	6.35412	-0.73432	-1.48647
F	6.63437	-2.07237	0.20235