

Table 1S. The z-matrices for reactants, hydrogen-bonded complexes and transition states involved in the reactions of 1,3,5-trioxane and 1,4-dioxane with OH radicals.

C₃H₆O₃

C

C	1	B1					
C	2	B2	1	A1			
H	2	B3	1	A2	3	D1	0
H	1	B4	2	A3	3	D2	0
H	1	B5	2	A4	3	D3	0
H	3	B6	2	A5	1	D4	0
H	3	B7	2	A6	1	D5	0
H	2	B8	1	A7	3	D6	0
O	1	B9	2	A8	3	D7	0
O	3	B10	2	A9	1	D8	0
O	1	B11	10	A10	2	D9	0

B1 2.29427208

B2 2.29491620

B3 1.08499294

B4 1.10102116

B5 1.08503004

B6 1.08496986

B7 1.10110873

B8 1.10106369

B9 1.40042199

B10 1.40035487

B11 1.40053960

A1 60.02406665

A2	142.78365356
A3	91.96252013
A4	142.75725416
A5	142.75234671
A6	91.95959518
A7	91.94529791
A8	35.00755331
A9	34.97881116
A10	111.16623205
D1	139.44192447
D2	91.16047437
D3	-139.32286949
D4	139.42425114
D5	-91.16658363
D6	-91.12328640
D7	-146.74201752
D8	146.71595508
D9	-57.14164098

HB1t

C

C	1	B1					
C	1	B2	2	A1			
H	2	B3	1	A2	3	D1	0
H	1	B4	3	A3	2	D2	0
H	1	B5	3	A4	2	D3	0
H	3	B6	1	A5	2	D4	0
H	3	B7	1	A6	2	D5	0
H	2	B8	1	A7	3	D6	0

O	1	B9	3	A8	2	D7	0
O	2	B10	1	A9	10	D8	0
O	1	B11	10	A10	2	D9	0
O	10	B12	1	A11	12	D10	0
H	13	B13	10	A12	1	D11	0

B1	2.30442936
B2	2.29606623
B3	1.08507862
B4	1.09986385
B5	1.08495456
B6	1.08460261
B7	1.10038646
B8	1.09928238
B9	1.40641076
B10	1.39865230
B11	1.39759995
B12	2.95017848
B13	0.97481572
A1	59.97596167
A2	142.68881402
A3	92.01638785
A4	142.96850248
A5	142.54963678
A6	92.08029589
A7	91.28935017
A8	90.12596661
A9	89.95967025
A10	110.67784860

A11	120.87143180
A12	21.13991171
D1	138.77427251
D2	-90.23633660
D3	139.79901213
D4	-138.95278394
D5	91.20478142
D6	-91.70478713
D7	18.92502967
D8	-127.31165594
D9	-58.18486079
D10	33.44438741
D11	50.01844042

TS1t

C							
C	1	B1					
C	2	B2	1	A1			
H	2	B3	1	A2	3	D1	0
H	1	B4	2	A3	3	D2	0
H	1	B5	2	A4	3	D3	0
H	3	B6	2	A5	1	D4	0
H	3	B7	2	A6	1	D5	0
H	2	B8	1	A7	3	D6	0
O	1	B9	2	A8	3	D7	0
O	3	B10	2	A9	1	D8	0
O	3	B11	2	A10	1	D9	0
O	3	B12	2	A11	1	D10	0
H	13	B13	3	A12	2	D11	0

B1	2.29029965
B2	2.29872552
B3	1.08455407
B4	1.09811917
B5	1.08480684
B6	1.08637398
B7	1.14780594
B8	1.09826522
B9	1.39831380
B10	1.38567166
B11	1.38941916
B12	2.68429729
B13	0.97053471
A1	60.35489400
A2	143.00289501
A3	91.72410960
A4	142.97250700
A5	143.81292305
A6	91.76224613
A7	91.54364985
A8	35.05945844
A9	34.95027533
A10	90.53428749
A11	88.72890435
A12	92.85428410
D1	137.86155074
D2	92.58556507
D3	-136.78022269

D4	140.95059128
D5	-92.11261298
D6	-91.84545714
D7	-144.17018723
D8	148.35758771
D9	16.71944458
D10	-83.96377741
D11	142.22072999

TS2t

C

C	1	B1				
C	1	B2	2	A1		
H	2	B3	1	A2	3	D1 0
H	1	B4	3	A3	2	D2 0
H	1	B5	3	A4	2	D3 0
H	3	B6	1	A5	2	D4 0
H	3	B7	1	A6	2	D5 0
H	2	B8	1	A7	3	D6 0
O	2	B9	1	A8	3	D7 0
O	2	B10	1	A9	10	D8 0
O	1	B11	10	A10	2	D9 0
O	2	B12	1	A11	12	D10 0
H	13	B13	2	A12	1	D11 0

B1	2.29799025
B2	2.29071727
B3	1.17947132
B4	1.09969912

B5	1.08469106
B6	1.08458447
B7	1.09976804
B8	1.10056500
B9	1.38932705
B10	1.38279667
B11	1.39670438
B12	2.49979470
B13	0.97009057
A1	59.97964852
A2	141.02265091
A3	92.03554378
A4	143.00995699
A5	142.93502673
A6	92.03285331
A7	96.97206108
A8	35.06867421
A9	90.58703984
A10	110.82696067
A11	130.95913015
A12	87.90202269
D1	137.34443136
D2	-91.62407418
D3	138.06121608
D4	-137.95422845
D5	91.79606368
D6	-94.22163869
D7	147.88006911
D8	-130.05191104

D9 -56.30543699
D10 117.74062608
D11 -12.33102079

HB2t

C

C	1	B1					
C	2	B2	1	A1			
H	2	B3	1	A2	3	D1	0
H	1	B4	2	A3	3	D2	0
H	1	B5	2	A4	3	D3	0
H	3	B6	2	A5	1	D4	0
H	2	B7	1	A6	3	D5	0
O	1	B8	2	A7	3	D6	0
O	3	B9	2	A8	1	D7	0
O	3	B10	2	A9	1	D8	0
O	11	B11	3	A10	2	D9	0
H	12	B12	11	A11	3	D10	0
H	12	B13	11	A12	3	D11	0

B1	2.28735751
B2	2.30189591
B3	1.08425705
B4	1.09615075
B5	1.08326684
B6	1.08031865
B7	1.09702593
B8	1.39498287
B9	1.36014759

B10	1.36647209
B11	2.82956164
B12	0.96217565
B13	0.95759263
A1	60.56782048
A2	143.00337977
A3	91.77298953
A4	143.80707582
A5	147.94747626
A6	91.44252830
A7	34.96187983
A8	34.53992762
A9	90.99565697
A10	142.41766606
A11	31.46656230
A12	136.68091566
D1	135.13342917
D2	94.17782176
D3	-134.63490284
D4	155.55313745
D5	-94.56472889
D6	-140.94820036
D7	153.22413643
D8	14.83888290
D9	-127.31303356
D10	-64.81743341
D11	-82.54194099

HB3t

C

C	1	B1					
C	1	B2	2	A1			
H	2	B3	1	A2	3	D1	0
H	1	B4	3	A3	2	D2	0
H	1	B5	3	A4	2	D3	0
H	3	B6	1	A5	2	D4	0
H	3	B7	1	A6	2	D5	0
H	2	B8	1	A7	3	D6	0
O	2	B9	1	A8	3	D7	0
O	2	B10	1	A9	10	D8	0
O	1	B11	10	A10	2	D9	0
O	10	B12	2	A11	1	D10	0
H	13	B13	10	A12	2	D11	0

B1 2.32824782

B2 2.28336615

B3 3.86644418

B4 1.09773498

B5 1.08461440

B6 1.08432028

B7 1.09812990

B8 1.08534500

B9 1.36615514

B10 1.35415526

B11 1.39180841

B12 2.87170584

B13 0.96267176

A1	60.35277724
A2	89.69790735
A3	91.66107901
A4	143.28679405
A5	143.00534408
A6	91.54594701
A7	120.36639916
A8	34.09383615
A9	90.26284546
A10	110.44507958
A11	91.73313874
A12	20.49515719
D1	-166.22789592
D2	-95.11762688
D3	133.89814812
D4	-133.86241370
D5	95.73126768
D6	-110.74719307
D7	154.34753218
D8	-140.59256210
D9	-51.46026029
D10	122.31773194
D11	140.02438738

C₄H₈O₂

C

C	1	B1			
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H	1	B2	2	A1	
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H	2	B3	1	A2	3	D1	0
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H	2	B4	1	A3	3	D2	0
H	1	B5	2	A4	4	D3	0
O	1	B6	2	A5	4	D4	0
C	1	B7	7	A6	2	D5	0
C	2	B8	1	A7	7	D6	0
O	9	B9	2	A8	1	D7	0
H	8	B10	1	A9	7	D8	0
H	9	B11	2	A10	1	D9	0
H	9	B12	2	A11	1	D10	0
H	8	B13	1	A12	7	D11	0

B1 2.32548370

B2 1.08920015

B3 1.08916829

B4 1.09735562

B5 1.09744577

B6 1.41302666

B7 1.51684793

B8 1.51676229

B9 1.41306516

B10 1.09730467

B11 1.08920195

B12 1.09735070

B13 1.08911751

A1 141.72628621

A2 141.72094545

A3 92.29339283

A4 92.30663258

A5 34.62985541

A6	110.48020086
A7	89.99710762
A8	110.48004823
A9	109.44891684
A10	110.92343538
A11	109.46867072
A12	110.95165409
D1	-0.02224719
D2	125.29063068
D3	-125.29884045
D4	-2.80573772
D5	-57.25466992
D6	-127.99926848
D7	-28.57815074
D8	-63.86124822
D9	-147.21680633
D10	92.43249801
D11	175.76056882

HB1d

C

C	1	B1				
H	1	B2	2	A1		
H	1	B3	2	A2	3	D1 0
H	2	B4	1	A3	4	D2 0
H	2	B5	1	A4	4	D3 0
O	1	B6	2	A5	5	D4 0
O	7	B7	1	A6	2	D5 0
H	8	B8	7	A7	1	D6 0

C	2	B9	1	A8	7	D7	0
H	10	B10	2	A9	1	D8	0
H	10	B11	2	A10	1	D9	0
C	1	B12	7	A11	2	D10	0
H	13	B13	1	A12	7	D11	0
H	13	B14	1	A13	7	D12	0
O	13	B15	1	A14	7	D13	0

B1 2.34705884

B2 1.09570974

B3 1.08863322

B4 1.08900541

B5 1.09564033

B6 1.41893823

B7 2.81777957

B8 0.97936037

B9 1.51572661

B10 1.08871520

B11 1.09706101

B12 1.51578687

B13 1.08874242

B14 1.09710901

B15 1.41231091

A1 92.14708423

A2 141.26222137

A3 141.06861168

A4 92.17369043

A5 34.24698855

A6 132.39993619

A7	4.49634989
A8	89.63320022
A9	110.84896751
A10	109.54958836
A11	109.94471128
A12	110.92711002
A13	109.55476790
A14	110.26927786
D1	-125.09784502
D2	-0.01955023
D3	-125.00153921
D4	2.92065838
D5	-178.73027042
D6	-19.59350520
D7	128.05386118
D8	147.44889851
D9	-92.20367714
D10	56.92590958
D11	-175.61903866
D12	64.00071615
D13	-57.03170104

TS1d

C

C	1	B1					
H	1	B2	2	A1			
H	1	B3	2	A2	3	D1	0
H	2	B4	1	A3	4	D2	0
H	2	B5	1	A4	4	D3	0

O	2	B6	1	A5	4	D4	0
O	2	B7	1	A6	7	D5	0
H	8	B8	2	A7	1	D6	0
C	2	B9	1	A8	7	D7	0
H	10	B10	2	A9	1	D8	0
H	10	B11	2	A10	1	D9	0
C	1	B12	7	A11	2	D10	0
H	13	B13	1	A12	7	D11	0
H	13	B14	1	A13	7	D12	0
O	10	B15	2	A14	1	D13	0

B1 2.32606776

B2 1.09554977

B3 1.08840431

B4 1.08911494

B5 1.15095535

B6 1.39472108

B7 2.62974489

B8 0.97018428

B9 1.51787674

B10 1.08835058

B11 1.09928944

B12 1.51529188

B13 1.08875889

B14 1.09753032

B15 1.40745452

A1 92.48703816

A2 140.64969781

A3 142.85039307

A4	92.27865404
A5	34.65356214
A6	86.99543799
A7	86.98583650
A8	90.12639634
A9	110.60036618
A10	108.62504666
A11	110.28258152
A12	110.75357423
A13	109.75569633
A14	111.21598215
D1	-125.84704403
D2	-1.59349005
D3	-125.14512950
D4	-4.34766066
D5	-111.30152500
D6	79.17657530
D7	131.67180620
D8	145.29134957
D9	-95.13660115
D10	56.10321112
D11	-176.47876661
D12	63.05642447
D13	25.93985145

TS2d

C

C	1	B1
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H	1	B2	2	A1		
H	1	B3	2	A2	3	D1 0
H	2	B4	1	A3	4	D2 0
H	2	B5	1	A4	4	D3 0
O	2	B6	1	A5	4	D4 0
O	2	B7	1	A6	7	D5 0
H	8	B8	2	A7	1	D6 0
C	2	B9	1	A8	7	D7 0
H	10	B10	2	A9	1	D8 0
H	10	B11	2	A10	1	D9 0
C	1	B12	7	A11	2	D10 0
H	13	B13	1	A12	7	D11 0
H	13	B14	1	A13	7	D12 0
O	13	B15	1	A14	7	D13 0

B1	2.32582061
B2	1.09609641
B3	1.08857139
B4	1.17413892
B5	1.09618958
B6	1.40006749
B7	2.50114642
B8	0.97036795
B9	1.51108825
B10	1.08787881
B11	1.09625212
B12	1.51627560
B13	1.08911557
B14	1.09705685

B15	1.41259163
A1	92.54772214
A2	141.06282689
A3	140.21003433
A4	96.49072986
A5	34.74750777
A6	127.72650142
A7	84.86750937
A8	90.70101532
A9	111.21621811
A10	109.33057386
A11	109.88922609
A12	110.82855533
A13	109.55603511
A14	110.31923169
D1	-125.48709330
D2	4.21515708
D3	-122.11536489
D4	-3.58014133
D5	12.14233605
D6	-6.76330320
D7	128.37147555
D8	147.05933294
D9	-92.11739983
D10	56.56374751
D11	-175.45468313
D12	64.10715484
D13	-56.93248474

HB2d

C

C	1	B1				
H	1	B2	2	A1		
H	1	B3	2	A2	3	D1 0
H	2	B4	1	A3	4	D2 0
H	2	B5	1	A4	4	D3 0
O	2	B6	1	A5	4	D4 0
O	7	B7	2	A6	1	D5 0
H	8	B8	7	A7	2	D6 0
C	2	B9	1	A8	7	D7 0
H	10	B10	2	A9	1	D8 0
H	10	B11	2	A10	1	D9 0
C	1	B12	7	A11	2	D10 0
H	13	B13	1	A12	7	D11 0
H	13	B14	1	A13	7	D12 0
O	13	B15	1	A14	7	D13 0

B1 2.34088916

B2 1.09309039

B3 1.08796399

B4 1.08167306

B5 2.79134937

B6 1.35959143

B7 2.99069749

B8 0.96146019

B9 1.49248849

B10 1.08854470

B11 1.10435643

B12	1.51247988
B13	1.08863506
B14	1.09774925
B15	1.41032807
A1	97.43891886
A2	137.31782817
A3	146.09866942
A4	80.01695825
A5	33.96003385
A6	86.67281345
A7	30.54507172
A8	90.84628568
A9	110.23326946
A10	110.18110761
A11	110.85461980
A12	110.18927039
A13	110.12163653
A14	110.11083926
D1	-129.96695351
D2	-29.18003901
D3	-110.57234597
D4	-17.26846135
D5	-88.42326635
D6	-122.48940360
D7	144.77332102
D8	142.40002531
D9	-98.64231753
D10	46.58003699
D11	-176.28746176

D12 63.59909387

D13 -57.85996088

HB3d

C

C	1	B1				
H	1	B2	2	A1		
H	1	B3	2	A2	3	D1 0
H	2	B4	1	A3	4	D2 0
H	2	B5	1	A4	4	D3 0
O	2	B6	1	A5	4	D4 0
O	7	B7	2	A6	1	D5 0
H	8	B8	7	A7	2	D6 0
C	2	B9	1	A8	7	D7 0
H	10	B10	2	A9	1	D8 0
H	10	B11	2	A10	1	D9 0
C	1	B12	7	A11	2	D10 0
H	13	B13	1	A12	7	D11 0
H	13	B14	1	A13	7	D12 0
O	13	B15	1	A14	7	D13 0

B1 2.34080773

B2 1.09252246

B3 1.08822926

B4 4.06100660

B5 1.08100439

B6 1.36535647

B7 2.85160199

B8 0.96427798

B9	1.49226781
B10	1.08841970
B11	1.10336117
B12	1.51443044
B13	1.08901326
B14	1.09639651
B15	1.41165768
A1	96.71890593
A2	137.72978735
A3	75.47340701
A4	145.97860565
A5	34.10705867
A6	99.20138925
A7	20.54766297
A8	90.73994431
A9	110.27768451
A10	109.90773857
A11	110.95882189
A12	109.96122430
A13	109.98290040
A14	109.89755148
D1	-129.66214621
D2	35.52493113
D3	-31.25035998
D4	-16.12284342
D5	103.20710641
D6	114.17204152
D7	143.05278849
D8	143.33036572

D9	-97.15056196
D10	47.47724381
D11	-175.92566393
D12	63.70743236
D13	-57.85716781

Table 2S. Vibrational frequencies and moments of inertia for the reactants and transition states of the reactions of C₃H₆O₃ and C₄H₈O₂ with OH radicals.

	The vibrational frequencies (cm ⁻¹)	The moments of inertia (amuÅ ²)
C ₃ H ₆ O ₃	302.7, 305.5, 482.6, 539.7, 540.7, 782.8, 995.0, 997.2, 1021.7, 1038.1, 1104.1, 1105.7, 1232.3, 1234.1, 1256.5, 1263.3, 1343.8, 1345.3, 1410.3, 1451.2, 1454.5, 1515.4, 1516.7, 136.7, 2994.8, 2995.2, 3009.1, 3175.9, 3186.7	94.7, 94.8, 170.5
TS1t	556.4i, 71.3, 110.9, 190.2, 298.6, 308.2, 471, 543.5, 544.3, 655.1, 787.4, 992.5, 997.9, 1018.9, 1041.6, 1049.1, 1113.0, 1216.7, 1240.1, 1244.3, 1274.1, 1343.8, 1355.2, 1409.6, 1429.4, 1449.6, 1457.9, 1521.8, 1538.3, 1751.5, 3045.7, 3070.7, 3170.1, 3186.4, 3188.8, 3774.4	253.7, 233.5, 151.5
TS2t	1105.1i, 69.1, 83.8, 183.3, 252.5, 283.6, 418.9, 535.8, 542.1, 750.1, 804.6, 906.7, 1009.2, 1014.7, 1037, 1059.7, 1096.2, 1109.1, 1204.2, 1244.2, 1246.4, 1282.0, 1333.9, 1344.9, 1380.2, 1431.6, 1452.7, 1517.7, 1531, 1547.9, 3017.8, 3022.8, 3033.4, 3181.7, 3191.3, 3788.2	100.5, 280.8, 350.9
C ₄ H ₈ O ₂	262.2, 288.3, 434.2, 446.5, 497.2, 619.2, 874.8, 878.2, 915.6, 931.6, 1055.6, 1079.9, 1116.6, 1159.2, 1199.9, 1202.7, 1251.4, 1299.6, 1331.8, 1342.6, 1370.3, 1404.3, 1421.1, 1437.3, 1489.5, 1492.5, 1500.7, 1507.1, 3020.5, 3025.5, 3031.5, 3034.5, 3119.8, 3121.2, 3121.8, 3122.6	98.5004 106.5638 182.4085
TS1d	626.9i, 69.3, 82.1, 185, 262.7, 275.3, 431.8, 448.4, 492, 595.9, 707.9, 874.1, 883.4, 913.8, 935.4, 1024.6, 1080.6, 1092.5, 1125.3, 1154.5, 1206.4, 1246.8, 1288.7, 1305.5, 1336.6, 1370.4, 1384.8, 1400.9, 1423.1, 1432.7, 1489.8, 1494.4, 1506.7, 1728.7, 3004.1, 3025.5, 3049.9, 3122, 3127.7, 3131.7, 3138.9, 3789	150.0917 252.2916 284.2557
TS2d	983.1i, 59.1, 94.5, 224.5, 259.7, 274.5, 393, 434.6, 491.2, 599.4, 749.9, 875.7, 881.4, 919, 946.7, 1012, 1056.9, 1087.6, 1134.2, 1158.6, 1192, 1216.4, 1259.6, 1292.5, 1317, 1330, 1345.8, 1393.7, 1400, 1428.1, 1492.9, 1500.6, 1506.3, 1607, 3024.5, 3039.3, 3039.7, 3058.1, 3123.9, 3127.4, 3134.8, 3792	110.9073 285.6299 360.0476

