Supplemental Material – Cartesian Coordinates for the Transition States

Cartesian Coordinates for TS-A

MacSPARTAN '14 Properties Program: (x86/Darwin) build 14.112

Use of molecular symmetry disabled

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C1	1.5067123	-0.1908755	0.2267111
2 O O5	-0.6291660	0.6946194	-0.2458321
3 O O1	2.0830133	1.2222961	-0.1878026
4 O O3	1.4551358	-0.3628039	1.3976400
5 C C2	-1.6483311	-0.0335051	-0.0370447
6 O O2	-1.6527834	-1.2786859	0.2002847
7 H H5	2.6050583	1.6240253	0.5466405
8 H H1	2.6568190	1.2070752	-0.9930680
9 C C3	-3.0060398	0.6778700	-0.0560419
10 H H2	-2.9201006	1.7083680	-0.4089703
11 H H3	-3.4289201	0.6845576	0.9563460
12 H H4	-3.7110694	0.1277219	-0.6887475
13 C C4	1.5130372	-1.0677738	-0.9661079

14	H	H6	2.5287577	-1.4652482	-1.0848638
15	H	H7	1.2146100	-0.5227799	-1.8605895
16	H	H8	0.8129762	-1.8814193	-0.7861665

Point Group = C1 Order = 1 Nsymop = 1

Cartesian Coordinates for TS-B

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
1	C	C1	1.3482610	0.2955468	-0.1640626
2	O	O5	-0.4218046	0.7683499	-0.2518585
3	O	O1	1.0995614	-1.4554053	-0.0287324
4	H	H3	0.0173171	-1.5184950	0.1283396
5	H	H4	1.2756349	-1.7436540	-0.9427412
6	O	O3	1.8865466	0.5719115	-1.1823006
7	C	C2	-1.4102005	-0.0155509	-0.0186989
8	O	O2	-1.3100599	-1.2455536	0.2461719
9	C	C3	-2.7817315	0.6210456	-0.0700605
10	H	H2	-2.8711979	1.3588606	0.7351262
11	H	H8	-2.9047630	1.1566256	-1.0166162
12	H	H7	-3.5578305	-0.1383630	0.0393986

13	C	C4	1.6459307	0.6737961	1.2552633
14	H	H1	2.6722867	0.3687646	1.4815146
15	H	H9	0.9598769	0.1927572	1.9519331
16	H	H10	1.5611696	1.7600580	1.3421539

Point Group = C1 Order = 1 Nsymop = 1

Cartesian Coordinates for TS-C

MacSPARTAN '14 Properties Program: (x86/Darwin) build 14.112

Use of molecular symmetry disabled

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
1	C C1	1.5708046	-0.1563626	0.1748439
2	O O5	-0.4606259	0.5449356	0.3522628
3	O O1	1.4116840	1.3495335	-0.7731322
4	O O3	2.1313993	0.0057298	1.1879202
5	C C2	-1.5526153	-0.1641562	0.1402621
6	O O2	-1.5813109	-1.3902625	0.1171247
7	H H5	1.8461968	2.0187232	-0.2109939
8	H H1	0.3882571	1.3196988	-0.4590503

9	C	C3	-2.8100815	0.6740845	-0.0533298
10	H	H2	-2.9403974	1.3562932	0.7937649
11	H	H3	-3.6843853	0.0269572	-0.1479821
12	H	H4	-2.7154287	1.2922287	-0.9546427
13	C	C4	1.3368748	-1.2679851	-0.7799188
14	H	H6	2.2476152	-1.8753100	-0.8164493
15	H	H7	1.0934729	-0.8866031	-1.7703181
16	H	H8	0.4856022	-1.8449622	-0.3988762

Point Group = C1 Order = 1 Nsymop = 1

Cartesian Coordinates for TS-D

MacSPARTAN '14 Properties Program: (x86/Darwin) build 14.112

Use of molecular symmetry disabled

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
1	C	C1	1.3679691	0.8136439	0.1153705
2	O	O5	-0.5263646	0.7894585	-0.4979855
3	O	O1	1.7475435	-0.5446516	-0.8685697
4	O	O3	1.7964419	1.8043385	-0.3537269

5	C	C2	-1.5612901	0.1889241	-0.0409966
6	O	O2	-1.5888211	-0.9384001	0.5190651
7	H	H4	-0.4694865	-1.9289937	0.1878960
8	O	O4	0.3528073	-2.4753780	-0.1026581
9	H	H5	1.4136487	-0.2280396	-1.7277641
10	H	H1	1.1743553	-1.4013705	-0.6051117
11	H	H2	0.0421039	-3.0986904	-0.7770319
12	C	C3	-2.8718546	0.9507644	-0.1868744
13	H	H3	-2.9178909	1.7328689	0.5811829
14	H	H7	-3.7249175	0.2807392	-0.0592420
15	H	H8	-2.9151256	1.4489823	-1.1596664
16	C	C4	1.2834942	0.3003723	1.5144077
17	H	H6	2.2781910	-0.0527764	1.8073923
18	H	H9	0.5543671	-0.4995553	1.6195650
19	H	H10	1.0019852	1.1416689	2.1523388

Point Group = C1 Order = 1 Nsymop = 1

Cartesian Coordinates for TS-E

MacSPARTAN '14 Properties Program: (x86/Darwin) build 14.112

Use of molecular symmetry disabled

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C1	1.1085983	0.0285733	0.0236151
2 O O1	0.8901559	1.1802013	-0.5038011
3 O O2	0.2062650	-0.7011213	0.5336282
4 C C2	-1.5790520	-0.2252166	0.0541148
5 O O3	-2.0547802	-1.1610685	-0.4568588
6 C C3	2.5290435	-0.4748405	0.0105542
7 H H1	3.2134997	0.3282063	0.2977401
8 H H3	2.7855044	-0.7805692	-1.0108059
9 H H4	2.6348361	-1.3319286	0.6775317
10 C C4	-1.5623780	1.1421601	0.3184782
11 H H2	-2.4902297	1.6395840	0.0351460
12 H H5	-0.2676082	1.3724439	-0.3294371
13 H H6	-1.1863985	1.4041137	1.3055063

Point Group = C1 Order = 1 Nsymop = 1

Cartesian Coordinates for Acetyl Cation

MacSPARTAN '14 Properties Program: (x86/Darwin) build 14.112

Use of molecular symmetry enabled

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
1	C C1	0.0000011	0.2133572	0.0000001
2	C C2	-0.0000002	-1.2293925	0.0000000
3	H H2	1.0411827	-1.5735931	0.0000000
4	H H1	-0.5205924	-1.5735909	-0.9016914
5	H H4	-0.5205924	-1.5735912	0.9016913
6	O O1	-0.0000004	1.3521234	-0.0000001

Point Group = CNV Order = 3 Nsymop = 6

Cartesian Coordinates for Acetate Anion

MacSPARTAN '14 Properties Program: (x86/Darwin) build 14.112

Use of molecular symmetry enabled

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
1	C C1	0.2133969	-0.0025352	0.0000000
2	O O1	0.8132642	1.1094939	0.0000000
3	O O2	0.6846748	-1.1761319	0.0000000
4	C C2	-1.3467466	0.0624439	0.0000000
5	H H1	-1.7075650	1.0956890	0.0000000
6	H H3	-1.7379244	-0.4610188	0.8804111
7	H H4	-1.7379244	-0.4610188	-0.8804111

Point Group = CS Order = 1 Nsymop = 2