

Correction to "Direct-Dynamics VTST Study of the [1,7] Hydrogen Shift in 7-Methylocta-1,3-(Z),5(Z)-triene. A Model System for the Hydrogen Transfer Reaction in Previtamin D₃" [The Journal of Physical Chemistry A **2007**, 111, 719–725. DOI: 10.1021/jp0665269]. S. Hosein Mousavipour, Antonio Fernández-Ramos,* Rubén Meana-Pañeda, Emilio Martínez-Nuñez, Saulo A. Vázquez, and Miguel A. Ríos*

We have found two important errors in our article related to the number of conformers of 7-methylocta-1,3(\mathbb{Z}),5(\mathbb{Z})-triene and to the optical isomers of most of those conformers. The errors are (1) the number of conformers of 7-methylocta-1,3-(Z),5(Z)-triene is thirteen, instead of seven, and (2) the transition state TS7 has one enantiomer, and therefore all the thermal rate constants should be multiplied by a factor of 2. As a result of these changes, the calculated thermal rate constant are now in much better agreement with experiment. The errors affect Tables 1-3 and 5, and Figures 1 and 3. In this document, we include the corrected version of Tables 1-3 and 5 and of Figures 1 and 3.

Table 1. Relative Classical Potential Energies (kcal/mol) and Main Distances (Å) and Angles (Degrees) of the Stationary Points Involved in the [1,7] Hydrogen Shift in 7-Methylocta-1,3(Z),5(Z)-triene Calculated at the MPWB1K/6-31+G(d,p) Level (Numbering as for Structure R1 in Figure 1)

R1 0.00 180.0 180.0 0.0 109.7 117.1 110.5 1.089 6.745 6.400 R2 2.78 -175.3 55.6 -80 109.1 117.1 110.5 1.088 4.302 3.519 R3 3.18 -39.9 117.1 0.0 109.6 117.3 110.5 1.089 5.612 5.330 R4 3.30 180.0 180.0 180.0 105.9 117.1 111.6 1.090 6.733 7.727 R5 6.41 -93.8 170.2 -173.3 106.0 117.3 111.6 1.090 5.616 6.374 R6 7.44 179.3 97.7 164.1 106.3 117.1 110.8 1.090 5.431 6.424 R7 7.70 36.9 5.88 -8.5 108.6 117.4 110.4 1.088 3.685 3.265 R8 1.158 2.99 74.0 126.6 105.1 117.1	structure	energy (gas)	$\phi_1^{\ a}$	$\phi_2^{\ a}$	ϕ_3^{a}	$\alpha_1^{\ a}$	α_2^a	α_3^{a}	$d(C_7 - H_{17})$	$d(C_1-C_7)$	$d(C_1 - H_{17})$
R3 3.18 -39.9 171.3 0.0 109.6 117.3 110.5 1.089 5.612 5.530 R4 3.30 180.0 180.0 180.0 105.9 117.1 111.6 1.090 6.793 7.727 R6 7.44 179.3 97.7 164.1 106.3 117.1 110.6 1.090 5.616 6.374 R7 7.70 36.9 38.8 -8.5 108.6 117.4 110.4 1.088 3.685 3.265 R8 11.158 29.9 74.0 128.0 105.1 117.3 110.4 1.088 3.685 3.265 R8 11.58 29.9 74.0 128.0 105.1 117.3 110.4 1.088 3.685 3.265 R8 11.58 29.9 -179.3 126.6 104.2 117.0 110.9 1.094 4.805 5.891 R1 1.0 3.8 1.2 1.18.1 110.5 117.3	R1	0.00	180.0	180.0	0.0	109.7	117.1	110.5	1.089	6.745	6.400
R4 3.30 180.0 180.0 180.0 105.9 117.1 111.6 1.090 6.793 7.727 R5 6.41 -39.8 170.2 -173.3 106.0 117.3 111.6 1.090 5.616 6.374 R6 7.44 179.3 39.7 164.1 106.3 117.4 110.6 1.091 5.431 6424 R7 7.70 36.9 58.8 -8.5 108.6 117.4 110.8 1.094 4.017 5.895 R9 6.79 -176.5 67.7 126.6 104.2 117.0 110.9 1.094 4.017 5.889 R10 3.80 -179.9 -179.3 126.5 105.1 117.1 110.3 1.094 4.805 5.881 R11 6.79 -37.6 166.4 -124.5 105.0 117.3 110.2 1.094 5.586 5.912 R12 6.85 -37.8 166.5 127.4 105.7 117.3	R2	2.78	-175.3	55.6	-8.0	109.1	117.1	110.2	1.088	4.302	3.519
RS 6.41 -39.8 170.2 -173.3 106.0 117.3 111.6 1.090 5.616 6.374 R6 7.44 179.3 97.7 164.1 106.3 117.1 110.8 1.091 5.431 6.424 R7 7.70 36.9 98.8 -8.5 108.6 117.4 110.4 1.088 3.685 3.265 R8 11.58 29.9 74.0 128.0 105.1 117.3 110.9 1.094 4.805 5.891 R10 3.80 -179.9 -179.3 126.5 105.1 117.1 110.3 1.094 6.888 7.533 R11 6.79 -37.6 1664 -124.5 105.1 117.3 110.3 1.094 6.888 7.533 R11 6.87 -37.8 166.5 127.4 105.7 117.3 110.3 1.094 5.88 6.393 R13 11.28 12.2 179.8 85.5 5.1 108.2	R3	3.18	-39.9	171.3	0.0	109.6	117.3	110.5	1.089	5.612	5.530
R6 7.44 179.3 97.7 164.1 106.3 117.1 110.8 1.091 5.431 6.424 R7 7.70 36.9 58.8 -8.5 108.6 117.4 110.4 1.088 3.685 3.265 R8 11.58 2.99 74.0 128.0 105.1 117.3 110.8 1.094 4.017 5.089 R9 6.79 -176.5 67.7 126.6 104.2 117.0 110.9 1.094 4.805 5.891 R10 3.80 -179.9 -179.3 126.5 105.0 117.3 110.5 1.094 6.88 7.533 R11 6.79 -3.76 166.5 127.4 105.7 117.3 110.5 1.094 5.886 5.912 R12 6.85 -37.8 166.5 127.4 105.7 117.3 110.2 1.094 5.886 6.912 R13 11.2 6.85 -37.8 166.5 5.1 108.2	R4	3.30	180.0	180.0	180.0	105.9	117.1	111.6	1.090	6.793	7.727
R7 7.70 36.9 58.8 -8.5 108.6 11.4 11.04 1.088 3.685 3.265 R8 11.58 29.9 74.0 128.0 105.1 117.3 110.8 1.094 4.017 5.089 R9 67.9 -176.5 67.7 126.6 104.2 117.0 110.9 1.094 4.805 5.891 R10 3.80 -179.9 -179.3 126.5 105.1 117.1 110.3 1.094 4.805 5.891 R11 6.79 -37.6 166.4 -124.5 105.0 117.3 110.5 1.094 5.586 5.912 R12 6.85 -37.8 166.5 127.4 105.7 117.3 110.2 1.094 5.586 5.912 R13 11.128 -24.5 82.9 -111.4 105.5 117.1 110.4 1.096 3.717 3.32 T51-3 6.08 -98.1 -178.7 -0.2 109.7 117.3 </td <td>R5</td> <td>6.41</td> <td>-39.8</td> <td>170.2</td> <td>-173.3</td> <td>106.0</td> <td>117.3</td> <td>111.6</td> <td>1.090</td> <td>5.616</td> <td>6.374</td>	R5	6.41	-39.8	170.2	-173.3	106.0	117.3	111.6	1.090	5.616	6.374
R8 11.58 29.9 74.0 128.0 105.1 117.3 110.8 1.094 4.017 5.089 R9 6.79 -176.5 67.7 126.6 104.2 117.0 110.9 1.094 4.805 5.891 R10 3.80 -179.9 -179.3 126.5 105.1 117.1 110.3 1.094 6.888 7.533 R11 6.79 -37.6 166.4 -124.5 105.0 117.3 110.2 1.094 5.586 5.912 R12 6.88 -37.8 166.5 127.4 105.7 117.3 110.2 1.094 5.586 5.912 R13 11.28 -24.5 82.9 -111.4 106.5 117.1 110.4 1.096 3.717 3.382 T51-2 4.82 179.8 98.5 5.1 108.5 117.1 110.4 1.096 3.717 3.382 T51-2 4.82 179.8 98.5 5.1 108.7 117.1<	R6	7.44	179.3	97.7	164.1	106.3	117.1	110.8	1.091	5.431	6.424
R9 6.79 -176.5 67.7 126.6 104.2 117.0 110.9 1.094 4.805 5.891 R10 3.80 -179.9 -179.3 126.5 105.1 117.1 110.3 1.094 6.888 7.533 R11 6.79 -37.6 166.4 -124.5 105.0 117.3 110.5 1.094 5.586 5.912 R12 6.85 -37.8 166.5 127.4 105.7 117.3 110.2 1.094 5.586 6.993 R13 11.28 -24.5 82.9 -111.4 106.5 117.1 110.4 1.096 3.717 3.382 T51-2 4.82 179.8 98.5 5.1 108.2 117.0 110.7 1.090 5.376 4.940 T51-3 6.08 -98.1 -178.7 -0.2 109.7 117.3 110.5 1.090 6.91 6.019 T51-10 4.55 179.7 177.6 89.1 107.3	R7	7.70	36.9	58.8	-8.5	108.6	117.4	110.4	1.088	3.685	3.265
R10 3.80 -179.9 -179.3 126.5 105.1 117.1 110.3 1.094 6.888 7.533 R11 6.79 -37.6 166.4 -124.5 105.0 117.3 110.5 1.094 5.586 5.912 R12 6.85 -37.8 166.5 127.4 105.7 117.3 110.2 1.094 5.586 6.393 R13 11.28 -24.5 82.9 -111.4 106.5 117.1 110.4 1.096 3.717 3.382 TS1-3 6.08 -98.1 -178.7 -0.2 109.7 117.3 110.5 1.089 6.191 6.019 TS1-3 6.08 -98.1 -178.7 -0.2 109.7 117.3 110.5 1.089 6.191 6.019 TS1-3 6.08 -98.1 -178.7 -0.2 109.7 117.3 110.5 1.089 6.191 6.019 TS1-10 4.55 179.7 177.6 89.1 107.3	R8	11.58	29.9	74.0	128.0	105.1	117.3	110.8	1.094	4.017	5.089
R11 6.79 -37.6 166.4 -124.5 105.0 117.3 110.5 1.094 5.586 5.912 R12 6.85 -37.8 166.5 127.4 105.7 117.3 110.2 1.094 5.588 6.393 R13 11.28 -24.5 82.9 -111.4 106.5 117.1 110.4 1.096 3.717 3.382 TS1-2 4.82 179.8 98.5 5.1 108.2 117.0 110.7 1.090 5.376 4.940 TS1-3 6.08 -98.1 -178.7 -0.2 109.7 117.3 110.5 1.089 6.191 6.019 TS1-3 6.08 -98.1 -178.7 -0.2 109.7 117.3 110.5 1.089 6.191 6.019 TS1-10 4.55 179.7 177.6 89.1 107.3 117.2 110.3 1.089 4.493 4.023 TS2-10 7.77 -179.1 96.8 -122.2 105.9	R9	6.79	-176.5	67.7	126.6	104.2	117.0	110.9	1.094	4.805	5.891
R12 6.85 -37.8 166.5 127.4 105.7 117.3 110.2 1.094 5.588 6.393 R13 11.28 -24.5 82.9 -111.4 106.5 117.1 110.4 1.096 3.717 3.382 TS1-2 4.82 179.8 98.5 5.1 108.2 117.0 110.7 1.090 5.376 4.940 TS1-3 6.08 -98.1 -178.7 -0.2 109.7 117.3 110.5 1.089 6.191 6.019 TS1-10 4.55 179.7 177.6 89.1 107.3 117.1 109.5 1.095 6.857 7.211 TS2-7 10.37 104.2 59.6 -3.7 108.7 117.2 110.3 1.095 6.857 7.211 TS2-10 7.77 -179.1 96.8 -122.2 105.9 117.1 110.6 1.094 5.510 5.540 TS3-1 7.82 -38.9 167.1 -81.6 107.2	R10	3.80	-179.9	-179.3	126.5	105.1	117.1	110.3	1.094	6.888	7.533
R13 11.28 −24.5 82.9 −111.4 106.5 117.1 110.4 1.096 3.717 3.382 TS1−2 4.82 179.8 98.5 5.1 108.2 117.0 110.7 1.090 5.376 4.940 TS1−3 6.08 −98.1 −178.7 −0.2 109.7 117.3 110.5 1.089 6.191 6.019 TS1−10 4.55 179.7 177.6 89.1 107.3 117.1 109.5 1.095 6.857 7.211 TS2−7 10.37 104.2 59.6 −3.7 108.7 117.2 110.3 1.089 4.493 4.023 TS2−10 7.77 −179.1 96.8 −122.2 108.2 117.1 110.6 1.094 5.510 5.540 TS3−1 7.87 8.81 18.7 93.5 6.2 108.2 117.1 110.6 1.094 5.51 5.540 TS3−12 7.35 −36.7 166.5 94.7 <	R11	6.79	-37.6	166.4	-124.5	105.0	117.3	110.5	1.094	5.586	5.912
TS1-2 4.82 179.8 98.5 5.1 108.2 117.0 110.7 1.090 5.376 4.940 TS1-3 6.08 -98.1 -178.7 -0.2 109.7 117.3 110.5 1.089 6.191 6.019 TS1-10 4.55 179.7 177.6 89.1 107.3 117.1 109.5 1.095 6.857 7.211 TS2-7 10.37 104.2 59.6 -3.7 108.7 117.2 110.3 1.089 4.493 4.023 TS2-10 7.77 -179.1 96.8 -122.2 105.9 117.1 110.6 1.094 5.510 5.540 TS3-7 8.81 18.7 93.5 62 108.2 117.1 110.6 1.094 5.510 5.540 TS3-11 7.82 -38.9 167.1 -81.6 107.2 117.3 109.6 1.095 5.557 6.247 TS4-5 9.36 -98.2 -179.0 179.7 106.0	R12	6.85	-37.8	166.5	127.4	105.7	117.3	110.2	1.094	5.588	6.393
TS1-3 6.08 -98.1 -178.7 -0.2 109.7 117.3 110.5 1.089 6.191 6.019 TS1-10 4.55 179.7 177.6 89.1 107.3 117.1 109.5 1.095 6.887 7.211 TS2-7 10.37 104.2 59.6 -3.7 108.7 117.2 110.3 1.089 4.493 4.023 TS2-10 7.77 -179.1 96.8 -122.2 105.9 117.1 110.6 1.094 5.510 5.540 TS3-7 8.81 18.7 93.5 6.2 108.2 117.1 110.6 1.094 5.510 5.540 TS3-1 7.82 -38.9 167.1 -81.6 107.2 117.3 109.5 1.094 5.614 5.651 TS4-5 9.36 -98.2 -179.0 179.7 106.0 177.3 117.3 109.6 1.095 5.557 6.247 TS4-5 9.36 -98.2 -179.0 179.7	R13	11.28	-24.5	82.9	-111.4	106.5	117.1	110.4	1.096	3.717	3.382
TS1-10 4.55 179.7 177.6 89.1 107.3 117.1 109.5 1.095 6.857 7.211 TS2-7 10.37 104.2 59.6 -3.7 108.7 117.2 110.3 1.089 4.493 4.023 TS2-10 7.77 -179.1 96.8 -122.2 105.9 117.1 110.6 1.094 5.510 5.540 TS3-7 8.81 18.7 93.5 6.2 108.2 117.1 110.6 1.094 5.510 5.540 TS3-11 7.82 -38.9 167.1 -81.6 107.2 117.3 109.5 1.094 5.614 5.651 TS3-12 7.35 -36.7 166.5 94.7 107.3 117.3 109.6 1.095 5.557 6.247 TS4-5 9.36 -98.2 -179.0 179.7 106.0 177.3 111.6 1.090 6.219 7.063 TS4-9 7.64 -179.6 97.9 133.2 105.6	TS1-2	4.82	179.8	98.5	5.1	108.2	117.0	110.7	1.090	5.376	4.940
TS2-7 10.37 104.2 59.6 -3.7 108.7 117.2 110.3 1.089 4.493 4.023 TS2-10 7.77 -179.1 96.8 -122.2 105.9 117.1 110.6 1.094 5.510 5.540 TS3-7 8.81 18.7 93.5 6.2 108.2 117.1 110.8 1.090 4.350 4.260 TS3-11 7.82 -38.9 167.1 -81.6 107.2 117.3 109.5 1.094 5.614 5.651 TS3-12 7.35 -36.7 166.5 94.7 107.3 117.3 109.6 1.095 5.557 6.247 TS4-5 9.36 -98.2 -179.0 179.7 106.0 177.3 111.6 1.090 6.219 7.063 TS4-9 7.64 -179.6 97.9 133.2 105.6 117.0 110.8 1.094 5.503 6.585 TS4-10 4.19 -179.7 -177.5 153.9 105.1	TS1-3	6.08	-98.1	-178.7	-0.2	109.7	117.3	110.5	1.089	6.191	6.019
TS2-10 7.77 -179.1 96.8 -122.2 105.9 117.1 110.6 1.094 5.510 5.540 TS3-7 8.81 18.7 93.5 6.2 108.2 117.1 110.8 1.090 4.350 4.260 TS3-11 7.82 -38.9 167.1 -81.6 107.2 117.3 109.5 1.094 5.614 5.651 TS3-12 7.35 -36.7 166.5 94.7 107.3 117.3 109.6 1.095 5.557 6.247 TS4-5 9.36 -98.2 -179.0 179.7 106.0 177.3 111.6 1.090 6.219 7.063 TS4-9 7.64 -179.6 97.9 133.2 105.6 117.0 110.8 1.094 5.503 6.585 TS4-10 4.19 -179.7 -177.5 153.9 105.1 117.1 110.8 1.091 6.830 7.666 TS5-12 7.47 -39.2 168.2 160.5 105.4 <td>TS1-10</td> <td>4.55</td> <td>179.7</td> <td>177.6</td> <td>89.1</td> <td>107.3</td> <td>117.1</td> <td>109.5</td> <td>1.095</td> <td>6.857</td> <td>7.211</td>	TS1-10	4.55	179.7	177.6	89.1	107.3	117.1	109.5	1.095	6.857	7.211
TS3-7 8.81 18.7 93.5 6.2 108.2 117.1 110.8 1.090 4.350 4.260 TS3-11 7.82 -38.9 167.1 -81.6 107.2 117.3 109.5 1.094 5.614 5.651 TS3-12 7.35 -36.7 166.5 94.7 107.3 117.3 109.6 1.095 5.557 6.247 TS4-5 9.36 -98.2 -179.0 179.7 106.0 177.3 111.6 1.090 6.219 7.063 TS4-9 7.64 -179.6 97.9 133.2 105.6 117.0 110.8 1.094 5.503 6.585 TS4-10 4.19 -179.7 -177.5 153.9 105.1 117.1 110.8 1.091 6.830 7.666 TS5-11 7.09 -37.1 166.9 -149.0 105.2 117.3 110.9 1.092 5.563 6.120 TS5-12 7.47 -39.2 168.2 160.5 105.4 <td>TS2-7</td> <td>10.37</td> <td>104.2</td> <td>59.6</td> <td>-3.7</td> <td>108.7</td> <td>117.2</td> <td>110.3</td> <td>1.089</td> <td>4.493</td> <td>4.023</td>	TS2-7	10.37	104.2	59.6	-3.7	108.7	117.2	110.3	1.089	4.493	4.023
TS3-11 7.82 -38.9 167.1 -81.6 107.2 117.3 109.5 1.094 5.614 5.651 TS3-12 7.35 -36.7 166.5 94.7 107.3 117.3 109.6 1.095 5.557 6.247 TS4-5 9.36 -98.2 -179.0 179.7 106.0 177.3 111.6 1.090 6.219 7.063 TS4-9 7.64 -179.6 97.9 133.2 105.6 117.0 110.8 1.094 5.503 6.585 TS4-10 4.19 -179.7 -177.5 153.9 105.1 117.1 110.8 1.091 6.830 7.666 TS5-11 7.09 -37.1 166.9 -149.0 105.2 117.3 110.9 1.092 5.563 6.120 TS5-12 7.47 -39.2 168.2 160.5 105.4 117.3 110.6 1.091 5.618 6.435 TS6-10 7.47 179.2 105.4 164.9 106	TS2-10	7.77	-179.1	96.8	-122.2	105.9	117.1	110.6	1.094	5.510	5.540
TS3-12 7.35 -36.7 166.5 94.7 107.3 117.3 109.6 1.095 5.557 6.247 TS4-5 9.36 -98.2 -179.0 179.7 106.0 177.3 111.6 1.090 6.219 7.063 TS4-9 7.64 -179.6 97.9 133.2 105.6 117.0 110.8 1.094 5.503 6.585 TS4-10 4.19 -179.7 -177.5 153.9 105.1 117.1 110.8 1.091 6.830 7.666 TS5-11 7.09 -37.1 166.9 -149.0 105.2 117.3 110.9 1.092 5.563 6.120 TS5-12 7.47 -39.2 168.2 160.5 105.4 117.3 110.6 1.091 5.618 6.435 TS6-10 7.47 179.2 105.4 164.9 106.5 117.1 110.7 1.091 5.605 6.602 TS7-8 11.65 9.0 83.6 125.1 105.6<	TS3-7	8.81	18.7	93.5		108.2	117.1	110.8	1.090	4.350	4.260
TS4-5 9.36 -98.2 -179.0 179.7 106.0 177.3 111.6 1.090 6.219 7.063 TS4-9 7.64 -179.6 97.9 133.2 105.6 117.0 110.8 1.094 5.503 6.585 TS4-10 4.19 -179.7 -177.5 153.9 105.1 117.1 110.8 1.091 6.830 7.666 TS5-11 7.09 -37.1 166.9 -149.0 105.2 117.3 110.9 1.092 5.563 6.120 TS5-12 7.47 -39.2 168.2 160.5 105.4 117.3 110.6 1.091 5.618 6.435 TS6-10 7.47 179.2 105.4 164.9 106.5 117.1 110.7 1.091 5.605 6.602 TS7-8 11.65 9.0 83.6 125.1 105.6 117.4 110.6 1.094 4.011 5.088 TS8-12 11.65 8.2 91.8 125.8 105.8 </td <td>TS3-11</td> <td>7.82</td> <td>-38.9</td> <td>167.1</td> <td>-81.6</td> <td>107.2</td> <td>117.3</td> <td>109.5</td> <td>1.094</td> <td>5.614</td> <td>5.651</td>	TS3-11	7.82	-38.9	167.1	-81.6	107.2	117.3	109.5	1.094	5.614	5.651
TS4-9 7.64 -179.6 97.9 133.2 105.6 117.0 110.8 1.094 5.503 6.585 TS4-10 4.19 -179.7 -177.5 153.9 105.1 117.1 110.8 1.091 6.830 7.666 TS5-11 7.09 -37.1 166.9 -149.0 105.2 117.3 110.9 1.092 5.563 6.120 TS5-12 7.47 -39.2 168.2 160.5 105.4 117.3 110.6 1.091 5.618 6.435 TS6-10 7.47 179.2 105.4 164.9 106.5 117.1 110.7 1.091 5.605 6.602 TS7-8 11.65 9.0 83.6 125.1 105.6 117.4 110.6 1.094 4.011 5.088 TS8-9 11.65 7.2 88.9 122.2 105.8 117.3 110.4 1.094 4.115 5.186 TS8-12 11.65 8.2 91.8 125.8 105.8	TS3-12	7.35	-36.7	166.5	94.7	107.3	117.3		1.095	5.557	
TS4-10 4.19 -179.7 -177.5 153.9 105.1 117.1 110.8 1.091 6.830 7.666 TS5-11 7.09 -37.1 166.9 -149.0 105.2 117.3 110.9 1.092 5.563 6.120 TS5-12 7.47 -39.2 168.2 160.5 105.4 117.3 110.6 1.091 5.618 6.435 TS6-10 7.47 179.2 105.4 164.9 106.5 117.1 110.7 1.091 5.605 6.602 TS7-8 11.65 9.0 83.6 125.1 105.6 117.4 110.6 1.094 4.011 5.088 TS8-9 11.65 7.2 88.9 122.2 105.8 117.3 110.4 1.094 4.115 5.186 TS8-12 11.65 8.2 91.8 125.8 105.8 117.2 110.4 1.094 4.199 5.262 TS10-12 9.76 -97.5 -178.0 125.2 105.3 </td <td></td> <td>9.36</td> <td>-98.2</td> <td>-179.0</td> <td>179.7</td> <td>106.0</td> <td>177.3</td> <td>111.6</td> <td>1.090</td> <td>6.219</td> <td>7.063</td>		9.36	-98.2	-179.0	179.7	106.0	177.3	111.6	1.090	6.219	7.063
TS5-11 7.09 -37.1 166.9 -149.0 105.2 117.3 110.9 1.092 5.563 6.120 TS5-12 7.47 -39.2 168.2 160.5 105.4 117.3 110.6 1.091 5.618 6.435 TS6-10 7.47 179.2 105.4 164.9 106.5 117.1 110.7 1.091 5.605 6.602 TS7-8 11.65 9.0 83.6 125.1 105.6 117.4 110.6 1.094 4.011 5.088 TS8-9 11.65 7.2 88.9 122.2 105.8 117.3 110.4 1.094 4.115 5.186 TS8-12 11.65 8.2 91.8 125.8 105.8 117.2 110.4 1.094 4.199 5.262 TS10-12 9.76 -97.5 -178.0 125.2 105.3 117.3 110.3 1.094 6.283 6.992 TS1-13 11.36 -27.0 95.9 -119.3 105.9 <td>TS4-9</td> <td>7.64</td> <td>-179.6</td> <td>97.9</td> <td>133.2</td> <td>105.6</td> <td>117.0</td> <td>110.8</td> <td>1.094</td> <td>5.503</td> <td></td>	TS4-9	7.64	-179.6	97.9	133.2	105.6	117.0	110.8	1.094	5.503	
TS5-12 7.47 -39.2 168.2 160.5 105.4 117.3 110.6 1.091 5.618 6.435 TS6-10 7.47 179.2 105.4 164.9 106.5 117.1 110.7 1.091 5.605 6.602 TS7-8 11.65 9.0 83.6 125.1 105.6 117.4 110.6 1.094 4.011 5.088 TS8-9 11.65 7.2 88.9 122.2 105.8 117.3 110.4 1.094 4.115 5.186 TS8-12 11.65 8.2 91.8 125.8 105.8 117.2 110.4 1.094 4.199 5.262 TS10-12 9.76 -97.5 -178.0 125.2 105.3 117.3 110.3 1.094 6.283 6.992 TS1-13 11.36 -27.0 95.9 -119.3 105.9 117.3 110.7 1.096 3.976 3.812 TS7 26.68 10.3 22.0 -64.5 100.0	TS4-10	4.19	-179.7	-177.5	153.9	105.1	117.1	110.8	1.091	6.830	7.666
TS6-10 7.47 179.2 105.4 164.9 106.5 117.1 110.7 1.091 5.605 6.602 TS7-8 11.65 9.0 83.6 125.1 105.6 117.4 110.6 1.094 4.011 5.088 TS8-9 11.65 7.2 88.9 122.2 105.8 117.3 110.4 1.094 4.115 5.186 TS8-12 11.65 8.2 91.8 125.8 105.8 117.2 110.4 1.094 4.199 5.262 TS10-12 9.76 -97.5 -178.0 125.2 105.3 117.3 110.3 1.094 6.283 6.992 TS11-13 11.36 -27.0 95.9 -119.3 105.9 117.3 110.7 1.096 3.976 3.812 TS7 26.68 10.3 22.0 -64.5 100.0 114.8 114.0 1.330 2.641 1.368 TS2 45.38 -127.1 27.7 -80.8 103.0	TS5-11	7.09	-37.1	166.9		105.2	117.3	110.9		5.563	6.120
TS7-8 11.65 9.0 83.6 125.1 105.6 117.4 110.6 1.094 4.011 5.088 TS8-9 11.65 7.2 88.9 122.2 105.8 117.3 110.4 1.094 4.115 5.186 TS8-12 11.65 8.2 91.8 125.8 105.8 117.2 110.4 1.094 4.199 5.262 TS10-12 9.76 -97.5 -178.0 125.2 105.3 117.3 110.3 1.094 6.283 6.992 TS11-13 11.36 -27.0 95.9 -119.3 105.9 117.3 110.7 1.096 3.976 3.812 TS7 26.68 10.3 22.0 -64.5 100.0 114.8 114.0 1.330 2.641 1.368 TS2 45.38 -127.1 27.7 -80.8 103.0 114.8 114.3 1.434 2.756 1.382 P1 0.60 -0.1 4.1 -96.7 76.7 <th< td=""><td>TS5-12</td><td>7.47</td><td></td><td>168.2</td><td>160.5</td><td>105.4</td><td>117.3</td><td>110.6</td><td>1.091</td><td>5.618</td><td></td></th<>	TS5-12	7.47		168.2	160.5	105.4	117.3	110.6	1.091	5.618	
TS8-9 11.65 7.2 88.9 122.2 105.8 117.3 110.4 1.094 4.115 5.186 TS8-12 11.65 8.2 91.8 125.8 105.8 117.2 110.4 1.094 4.199 5.262 TS10-12 9.76 -97.5 -178.0 125.2 105.3 117.3 110.3 1.094 6.283 6.992 TS11-13 11.36 -27.0 95.9 -119.3 105.9 117.3 110.7 1.096 3.976 3.812 TS7 26.68 10.3 22.0 -64.5 100.0 114.8 114.0 1.330 2.641 1.368 TS2 45.38 -127.1 27.7 -80.8 103.0 114.8 114.3 1.434 2.756 1.382 P1 0.60 -0.1 4.1 -96.7 76.7 109.1 115.1 3.016 3.514 1.091		7.47	179.2		164.9	106.5	117.1			5.605	
TS8-12 11.65 8.2 91.8 125.8 105.8 117.2 110.4 1.094 4.199 5.262 TS10-12 9.76 -97.5 -178.0 125.2 105.3 117.3 110.3 1.094 6.283 6.992 TS11-13 11.36 -27.0 95.9 -119.3 105.9 117.3 110.7 1.096 3.976 3.812 TS7 26.68 10.3 22.0 -64.5 100.0 114.8 114.0 1.330 2.641 1.368 TS2 45.38 -127.1 27.7 -80.8 103.0 114.8 114.3 1.434 2.756 1.382 P1 0.60 -0.1 4.1 -96.7 76.7 109.1 115.1 3.016 3.514 1.091	TS7-8	11.65		83.6	125.1	105.6	117.4	110.6	1.094	4.011	5.088
TS10-12 9.76 -97.5 -178.0 125.2 105.3 117.3 110.3 1.094 6.283 6.992 TS11-13 11.36 -27.0 95.9 -119.3 105.9 117.3 110.7 1.096 3.976 3.812 TS7 26.68 10.3 22.0 -64.5 100.0 114.8 114.0 1.330 2.641 1.368 TS2 45.38 -127.1 27.7 -80.8 103.0 114.8 114.3 1.434 2.756 1.382 P1 0.60 -0.1 4.1 -96.7 76.7 109.1 115.1 3.016 3.514 1.091	TS8-9	11.65	7.2	88.9		105.8	117.3	110.4	1.094	4.115	
TS11-13 11.36 -27.0 95.9 -119.3 105.9 117.3 110.7 1.096 3.976 3.812 TS7 26.68 10.3 22.0 -64.5 100.0 114.8 114.0 1.330 2.641 1.368 TS2 45.38 -127.1 27.7 -80.8 103.0 114.8 114.3 1.434 2.756 1.382 P1 0.60 -0.1 4.1 -96.7 76.7 109.1 115.1 3.016 3.514 1.091	TS8-12					105.8	117.2	110.4			
TS7 26.68 10.3 22.0 -64.5 100.0 114.8 114.0 1.330 2.641 1.368 TS2 45.38 -127.1 27.7 -80.8 103.0 114.8 114.3 1.434 2.756 1.382 P1 0.60 -0.1 4.1 -96.7 76.7 109.1 115.1 3.016 3.514 1.091	TS10-12				125.2	105.3	117.3	110.3	1.094	6.283	
TS2 45.38 -127.1 27.7 -80.8 103.0 114.8 114.3 1.434 2.756 1.382 P1 0.60 -0.1 4.1 -96.7 76.7 109.1 115.1 3.016 3.514 1.091											
P1 0.60 -0.1 4.1 -96.7 76.7 109.1 115.1 3.016 3.514 1.091											
P2 0.67 176.8 4.7 -65.1 101.0 108.2 115.5 4.524 4.598 1.090											
$a = \phi(C_1 - C_2 - C_3)$ $\phi_1 = \phi(C_2 - C_3 - C_4)$ $\phi_2 = \phi(C_2 - C_3 - C_4)$ $\phi_3 = \phi(C_3 - C_4 - C_5)$ $\phi_4 = \phi(C_4 - C_4 - C_4)$ $\phi_4 = \phi(C_4 - C_4 - C_4)$ $\phi_5 = \phi(C_4 - C_4 - C$											

 $^{^{}a}\phi_{1}=\phi(C_{1}-C_{2}-C_{3}-C_{4}), \phi_{2}=\phi(C_{3}-C_{4}-C_{5}-C_{6}), \phi_{3}=\phi(C_{5}-C_{6}-C_{7}-C_{17}), \alpha_{1}=\alpha(C_{6}-C_{7}-H_{17}), \alpha_{2}=\alpha(H_{10}-C_{1}-H_{11}), \alpha_{3}=\alpha(C_{8}-C_{7}-C_{9}).$



Line 4 of the Abstract, "seven conformers" should be "thirteen conformers."

Table 2. Calculated (Columns 2, 3 and 4) and Experimental (Column 5) Thermal Rate Constants (s^{-1}) for the [1,7] Hydrogen (and Deuterium) Shift in 7-Methylocta-1,3(Z),5(Z)-triene

_				•	
	T (K)	TST	CVT	$\text{CVT}/\mu\text{OMT}$	\exp^a
			k_{H}		
	298.2	1.48×10^{-7}	1.45×10^{-7}	1.09×10^{-6}	
	333.2	1.02×10^{-5}	1.00×10^{-5}	4.80×10^{-5}	5.6×10^{-5}
	348.2	4.82×10^{-5}	4.72×10^{-5}	1.96×10^{-4}	2.14×10^{-4}
	368.2	3.12×10^{-4}	3.06×10^{-4}	1.08×10^{-3}	1.16×10^{-3}
	388.2	1.67×10^{-3}	1.63×10^{-3}	5.03×10^{-3}	5.51×10^{-2}
	400.0	4.13×10^{-3}	4.05×10^{-3}	1.16×10^{-2}	
			$k_{ m D}$		
	298.2	3.23×10^{-8}	3.20×10^{-8}	1.55×10^{-7}	
	333.2	2.60×10^{-6}	2.60×10^{-6}	8.72×10^{-6}	8.0×10^{-6}
	348.2	1.30×10^{-5}	1.29×10^{-5}	3.84×10^{-5}	3.3×10^{-5}
	368.2	9.03×10^{-5}	8.94×10^{-5}	2.33×10^{-4}	2.21×10^{-4}
	388.2	5.13×10^{-4}	5.08×10^{-4}	1.19×10^{-3}	1.21×10^{-3}
	400.0	1.31×10^{-3}	1.30×10^{-3}	2.89×10^{-3}	
a	From ref	f 8.			

Table 3. Arrhenius Parameters (Activation Energy, E_a , kcal·mol⁻¹, and Logarithm of the Preexponential Factor, $\log(A/s^{-1})$), for [1,7] Sigmatropic Hydrogen (and Deuterium) Shift Reactions^a

	[1,7]	H shift	[1,7] D shift		
	$E_{\rm a}$	$\log A$	$E_{\rm a}$	$\log A$	
CVT	23.81	10.62	24.65	10.58	
CVT/ZCT	22.70	10.27	23.60	10.24	
$\text{CVT}/\mu\text{OMT}$	21.74	9.94	22.97	10.00	
Baldwin and Reddy ⁸	21.5	9.8	23.5	10.3	

^a The fit to the calculated values included only temperatures in the interval 333.2—388.2 K to get a more reliable comparison with the experimental data.

The first paragraph of section 3 that describes the conformers should be replaced by the following paragraph: "Figure 1 shows the thirteen possible conformers of 7-methylocta-1,3(Z),5(Z)triene. According to the MPWB1K/DIDZ calculations, all the conformers can be characterized by specifying the value of the three dihedral angles, ϕ_1 , ϕ_2 , and ϕ_3 , which are defined as the torsions about the C_2-C_3 , C_4-C_5 , and C_6-C_7 atoms, respectively (Figure 1 and Table 1). R1 is the most stable conformer with ϕ_1 and ϕ_2 in s-trans, s-trans configuration. According to the value of these two dihedral angles, all equilibrium structures can be divided in four groups, and in each of them the rotation about ϕ_3 leads to the different conformers. The first group includes all the s-trans, s-trans configurations, i.e., R1, R4, and R10. The second group involves the s-cis,s-trans structures, R3, R5, R11, and R12. The third group of conformers arises when ϕ_1 is kept in s-trans configuration and ϕ_2 takes values between 55° and 98° (conformers R2, R6, and R9). The fourth group includes the R8, R13, and R7 conformations. They are obtained by rotation of both ϕ_1 and ϕ_2 with respect to the s-trans, s-trans configuration. With the exception of R1 and R4, which are achiral (both of them have a plane of symmetry), all the other conformers are chiral and have enantiomers. Some of the key distances and angles of the thirteen conformers, together with some of the transition states involved in the interconversion between the conformers are listed in Table 1."

Table 5. Factors in the KIEs^a

T (K)	$\eta_{ m var}$	$\eta_{ m int}$	$\eta_{ m cl}$	$\eta_{ ext{tun}}^{ ext{ZCT}}$	$\eta_{ m tun}^{\mu m OMT}$	$\eta_{ m calc}$	$\eta_{ m exp}$
298.2	0.99	4.59	4.54	1.09	1.55	7.0	
333.2	0.98	3.92	3.84	1.08	1.43	5.5	$7.0^{+1.3}_{-0.8}$
348.2	0.99	3.70	3.67	1.08	1.40	5.1	$6.5^{+0.7}_{-1.1}$
368.2	0.99	3.46	3.42	1.07	1.35	4.6	$5.2^{+0.9}_{-0.6}$
388.2	0.99	3.25	3.22	1.07	1.32	4.2	4.6 ± 0.6
400.0	0.99	3.14	3.11	1.06	1.29	4.0	

^a The classical, $\eta_{\rm cl}$, and total, $\eta_{\rm calc}$ KIEs are given by eqs 11 and 9, respectively. The experimental KIEs, $\eta_{\rm exp}$, are taken from Baldwin and Reddy⁸ considering a deviation of $E_{\rm a}^{\rm D}-E_{\rm a}^{\rm H}$) 0.1 kcal·mol⁻¹. The factors $\eta_{\rm tun}^{\rm ZCT}$ and $\eta_{\rm tun}^{\rm uOMT}$ are also listed for comparison.

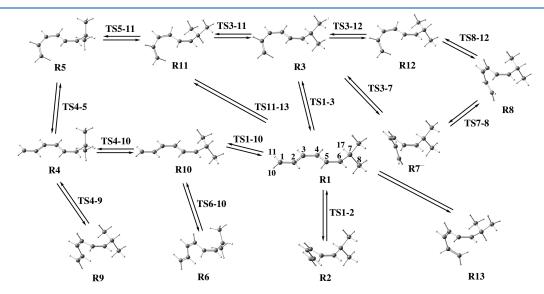


Figure 1. Thirteen conformers of the 7-Methylocta-1,3(Z),5(Z)-triene. The arrows between two structures indicate that there is a transition state connecting them (not all of them are shown). Details about the geometries and relative energies of the conformers and the transition states are given in Table 1.

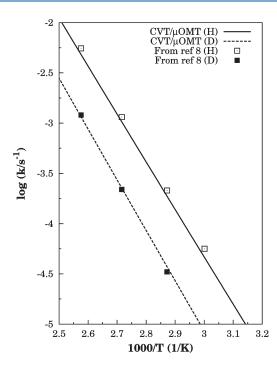


Figure 3. Thermal rate constants calculated in this work by the CVT/ μ OMT method for the hydrogen (solid line) and deuterium (dashed line) shift reactions of 7-methylocta-1,3(Z),5(Z)-triene. The experimental values (squares) are also plotted for comparison.

Equation 14 should be replaced by

$$k^{\rm CVT}(T) = \frac{2}{\beta h} \frac{Q^{\rm GT}(T, s_*^{\rm CVT})}{\sum_{i=1}^{13} (n^{\rm R_i}/\sigma^{\rm R_i}) Q^{\rm R_i}(T) e^{-\beta \Delta E_{\rm R_i}}} \exp[-\beta V_{\rm MEP}(s_*^{\rm CVT})]$$
(14)

The first sentence after eq 14 should be replaced by "where the sum runs over the thirteen conformers (i=1,...,13), with $Q^{\mathbf{R}_i}(T)$ and $\Delta E_{\mathbf{R}_i}$ being the partition function of conformer \mathbf{R}_i and the relative energy of conformer \mathbf{R}_i regarding the most stable conformer, respectively. The number two in the numerator takes into account that **TS7** has one enantiomer. The enantiomers of \mathbf{R}_i are specified in $n^{\mathbf{R}_i}$, thus $n^{\mathbf{R}_i}=2$ for all conformers except for i=1,4."

On page 722, the sentence "The CVT/ μ OMT values ..." should be replaced by "The CVT/ μ OMT values are in good agreement with the experimetal ones for both the hydrogen and deuterium transfer."

On page 723, the numerical values in the sentence "When the contribution of the ZCT ... " are slightly different: 0.06 should replace 0.04, 0.39 should replace 0.41, and 1.23 should replace 1.29.

On page 724 (third line of the second parapraph), 3.84 should replace 3.73.

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