Theoretical and Kinetic Study of the Reaction of Ethyl Methyl Ketone with HO_2 for T=600−1,600 K, Part II: Addition Reaction Channels

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Supporting Information

TABLE S1. T1 diagnostics, rotational symmetry number (σ), optical isomers (m) and optimized Cartesian coordinates of important species involved in EMK + HO_2 reaction, computed at the B3LYP/6-311+G(d,p) level. Gaussian 09[1] and MOLPRO[2] are used in the geometry and energy calculations.

Species	T1 diagnostics	σ	m	Cartesian coordinates, angstroms			
				Atomic number	X	Y	Z
EMK	1.84E-06	9	1	6	0.528114000	0.169726000	-0.012743000
				8	0.414861000	1.374309000	-0.015171000
				6	1.889791000	-0.502679000	0.022628000
				1	1.975373000	-1.261571000	-0.760585000
				1	2.672027000	0.245862000	-0.096361000
				1	2.024543000	-1.014890000	0.981173000
				6	-0.684292000	-0.754094000	-0.039154000
				1	-0.615343000	-1.356737000	-0.954494000
				1	-0.580402000	-1.474279000	0.782406000
				6	-2.020158000	-0.020344000	0.032091000
				1	-2.852804000	-0.726429000	-0.012102000
				1	-2.102800000	0.551985000	0.958221000
				1	-2.120211000	0.685932000	-0.793816000
HO_2	7.16E-04	1	1	8	0.055283000	0.718471000	0.000000000
				8	0.055283000	-0.609632000	0.000000000
				1	-0.884535000	-0.870716000	0.000000000
RO_2	4.64E-04	9	2	6	-1.042317000	1.563125000	-0.275432000
				6	-0.120417000	0.402057000	0.073206000

				6	1.316603000	0.567629000	-0.398121000
				6	2.237447000	-0.594075000	-0.018969000
				8	-0.155020000	0.070090000	1.410880000
				1	-2.068162000	1.317548000	0.008732000
				1	-1.018651000	1.779453000	-1.345163000
				1	-0.727883000	2.450146000	0.277580000
				1	1.688695000	1.504134000	0.029259000
				1	1.293857000	0.703331000	-1.483643000
				1	3.251292000	-0.406138000	-0.380053000
				1	1.889165000	-1.530224000	-0.460069000
				1	2.274105000	-0.722659000	1.063221000
				1	-1.039221000	-0.288787000	1.582228000
				8	-1.678970000	-1.336863000	-0.128275000
				8	-0.652397000	-0.788129000	-0.729630000
α_p-QOOH	1.51E-04	3	2	6	-0.916937000	1.564729000	-0.394226000
				6	-0.087273000	0.395536000	0.038507000
				6	1.366956000	0.493040000	-0.457470000
				6	2.250199000	-0.681711000	-0.026049000
				8	-0.069684000	0.259215000	1.432965000
				1	-2.476716000	-0.688900000	-0.701336000
				1	-1.148027000	1.702414000	-1.444174000
				1	-1.146119000	2.353136000	0.310237000
				1	1.764460000	1.433168000	-0.064604000
				1	1.344131000	0.583578000	-1.547033000
				1	3.276248000	-0.523029000	-0.368491000
				1	1.888532000	-1.620950000	-0.446441000
				1	2.258030000	-0.776159000	1.060257000
				1	-0.960418000	-0.015107000	1.686646000
				8	-1.902099000	-1.080257000	-0.028087000
				8	-0.587942000	-0.813672000	-0.586083000
α_s-QOOH	1.99E-04	9	2	6	-1.169693000	-1.128508000	0.903515000
				6	-0.127155000	-0.450551000	0.025683000
				6	0.993103000	0.178302000	0.784412000
				6	2.253593000	0.577139000	0.102485000
				8	0.417505000	-1.321410000	-0.931006000
				1	-1.961061000	-1.548841000	0.277264000
				1	-1.622110000	-0.412640000	1.589627000
				1	-0.700567000	-1.933587000	1.472533000
				1	0.874117000	0.319741000	1.851708000
				1	-0.863812000	2.240065000	-0.005268000
				1	2.766402000	1.380503000	0.638164000
				1	2.059037000	0.897784000	-0.924664000
				1	2.955779000	-0.266692000	0.032398000
				1	-0.311133000	-1.641054000	-1.477494000
				8	-1.496370000	1.508629000	-0.020789000
				8	-0.783102000	0.551085000	-0.842060000
TS1	4.73E-04	9	2	6	-0.926116000	1.798261000	-0.201034000
				6	-0.056223000	0.635658000	0.204950000
				6	1.343088000	0.573989000	-0.370987000
				6	2.124513000	-0.685106000	-0.001263000
				8	-0.307116000	0.041595000	1.315353000
				1	-1.958969000	1.614163000	0.094466000
				1	-0.874015000	1.990787000	-1.273637000
				1	-0.576162000	2.692999000	0.326678000
				1	1.863842000	1.465740000	0.007115000

				1	1.282077000	0.700878000	-1.455883000
				1	3.145107000	-0.628125000	-0.385959000
				1	1.653814000	-1.574916000	-0.424307000
				1	2.169286000	-0.809670000	1.081512000
				1	-0.899168000	-0.912411000	0.965477000
				8	-1.346223000	-1.568844000	0.014120000
				8	-0.936334000	-0.782283000	-0.920154000
TS2	3.00E-04	3	2	6	-1.158135000	1.271297000	-0.420196000
				6	-0.073470000	0.289428000	0.056441000
				6	1.320536000	0.540947000	-0.507081000
				6	2.352433000	-0.502939000	-0.066679000
				8	-0.000213000	0.267296000	1.455137000
				1	-2.054773000	0.249089000	-0.277769000
				1	-1.180666000	1.484205000	-1.487614000
				1	-1.370738000	2.118515000	0.225412000
				1	1.625190000	1.538817000	-0.176220000
				1	1.240183000	0.569401000	-1.596704000
				1	3.334792000	-0.260259000	-0.478839000
				1	2.071576000	-1.498650000	-0.415273000
				1	2.429359000	-0.532030000	1.020565000
				1	-0.827375000	-0.118105000	1.772355000
				8	-1.936780000	-0.944546000	-0.109852000
				8	-0.552473000	-0.965673000	-0.465387000
TS3	2.74E-04	9	2	6	-1.655453000	-0.454173000	0.860385000
				6	-0.409917000	-0.349453000	-0.009681000
				6	0.863963000	0.005605000	0.779405000
				6	2.182426000	-0.255738000	0.108649000
				8	-0.191222000	-1.486682000	-0.780549000
				1	-2.529706000	-0.630868000	0.226974000
				1	-1.813605000	0.480435000	1.399266000
				1	-1.560209000	-1.274426000	1.575117000
				1	0.824205000	-0.211460000	1.846442000
				1	0.532230000	1.311566000	0.590415000
				1	3.002066000	0.214024000	0.657534000
				1	2.178145000	0.113241000	-0.918655000
				1	2.380830000	-1.333927000	0.067269000
				1	-1.037508000	-1.802287000	-1.116880000
				8	-0.251737000	1.900541000	-0.126139000
				8	-0.539861000	0.768172000	-0.938315000
TS2a	7.22E-04	3	2	6	-0.882414000	1.685075000	-0.340898000
				6	-0.433414000	0.484729000	0.146136000
				6	1.678581000	0.394098000	-0.666889000
				6	2.352547000	-0.715399000	0.073313000
				8	-0.215927000	0.328916000	1.480395000
				1	-2.559155000	-0.753360000	-0.752362000
				1	-1.164961000	1.762006000	-1.380366000
				1	-0.795310000	2.580527000	0.257356000
				1	1.965244000	1.409564000	-0.414238000
				1	1.449043000	0.235692000	-1.714942000
				1	3.406842000	-0.808561000	-0.228296000
				1	1.874811000	-1.678229000	-0.124563000
				1	2.355071000	-0.532972000	1.152417000
				1	-0.008170000	-0.599957000	1.633984000
				8	-1.981325000	-1.230092000	-0.138213000
				8	-0.654650000	-0.687039000	-0.554551000

TS2b	**5.26E-04**	**3**	**2**	**6**	**-0.661542000**	**1.727799000**	**-0.359236000**
				6	**0.111124000**	**0.677464000**	**0.151891000**
				6	**1.507880000**	**0.422030000**	**-0.362695000**
				6	**2.066863000**	**-0.963309000**	**-0.033723000**
				8	**-0.095910000**	**0.239159000**	**1.417864000**
				1	**-2.684755000**	**-0.789441000**	**-0.378071000**
				1	**-0.444879000**	**2.142675000**	**-1.333627000**
				1	**-1.560433000**	**2.046771000**	**0.153363000**
				1	**2.152070000**	**1.196725000**	**0.072189000**
				1	**1.503581000**	**0.595574000**	**-1.442546000**
				1	**3.085313000**	**-1.059187000**	**-0.418611000**
				1	**1.448356000**	**-1.742009000**	**-0.480130000**
				1	**2.090322000**	**-1.124171000**	**1.044860000**
				1	**-1.008802000**	**-0.095099000**	**1.466015000**
				8	**-1.875982000**	**-1.107262000**	**0.046900000**
				8	**-0.868949000**	**-0.676364000**	**-0.847373000**
TS2c	**1.07E-03**	**3**	**2**	**6**	**-0.873412000**	**1.471612000**	**-0.508656000**
				6	**-0.052016000**	**0.359972000**	**-0.435221000**
				6	**1.449295000**	**0.432784000**	**-0.553737000**
				6	**2.214648000**	**-0.607513000**	**0.269570000**
				8	**-0.433974000**	**0.263401000**	**1.610033000**
				1	**-1.715545000**	**-0.740555000**	**0.736611000**
				1	**-1.941236000**	**1.362289000**	**-0.615864000**
				1	**-0.437945000**	**2.456040000**	**-0.414998000**
				1	**1.749358000**	**1.445532000**	**-0.274799000**
				1	**1.686372000**	**0.318850000**	**-1.619081000**
				1	**3.290220000**	**-0.461807000**	**0.144111000**
				1	**1.967042000**	**-1.620749000**	**-0.049030000**
				1	**1.957870000**	**-0.508918000**	**1.323716000**
				1	**-0.679015000**	**1.135388000**	**1.951292000**
				8	**-1.862217000**	**-1.031762000**	**-0.198817000**
				8	**-0.492335000**	**-0.897539000**	**-0.637928000**
TS2d	**5.17E-04**	**3**	**2**	**6**	**-0.817099000**	**1.579042000**	**-0.055229000**
				6	**0.015793000**	**0.344130000**	**0.122625000**
				6	**1.497685000**	**0.555255000**	**-0.224027000**
				6	**2.332010000**	**-0.724654000**	**-0.165242000**
				8	**-0.084928000**	**-0.232188000**	**1.392747000**
				1	**-2.292378000**	**-1.624324000**	**-0.585107000**
				1	**-0.489862000**	**2.364459000**	**-0.726248000**
				1	**-1.858378000**	**1.536978000**	**0.230307000**
				1	**1.865712000**	**1.292705000**	**0.498361000**
				1	**1.552561000**	**1.012913000**	**-1.215259000**
				1	**3.384720000**	**-0.499396000**	**-0.352730000**
				1	**2.002969000**	**-1.446127000**	**-0.916089000**
				1	**2.247602000**	**-1.191956000**	**0.816429000**
				1	**-0.990095000**	**-0.581987000**	**1.422160000**
				8	**-2.298273000**	**-0.743547000**	**-0.182902000**
				8	**-0.565947000**	**-0.447503000**	**-0.864918000**
TS3a	**7.26E-04**	**9**	**2**	**6**	**0.239115000**	**1.493992000**	**1.322423000**
				6	**-0.002797000**	**0.055368000**	**-0.403900000**
				6	**-0.834234000**	**-0.864860000**	**0.167859000**
				6	**-2.315068000**	**-0.681736000**	**0.256683000**
				8	**-0.449204000**	**0.929062000**	**-1.347503000**
				1	**0.947696000**	**2.165091000**	**0.846222000**
				1	**0.645056000**	**0.887287000**	**2.121668000**

				1	-0.765687000	1.875444000	1.463724000
				1	-0.366021000	-1.665745000	0.723481000
				1	2.110999000	-1.766576000	-0.059049000
				1	-2.838609000	-1.588671000	-0.065300000
				1	-2.652696000	0.142673000	-0.371692000
				1	-2.638427000	-0.482413000	1.287094000
				1	0.128890000	1.701193000	-1.342064000
				8	1.952876000	-0.935906000	0.412137000
				8	1.359666000	-0.153765000	-0.647443000
TS3b	**3.31E-04**	**3**	**2**	6	0.475781000	1.124533000	1.194590000
				6	0.029198000	0.352066000	-0.044337000
				6	-0.899628000	-0.787019000	0.284986000
				6	-2.171144000	-0.865858000	-0.106383000
				8	-0.569849000	1.175720000	-0.995075000
				1	1.173392000	1.914282000	0.899401000
				1	0.985852000	0.469141000	1.900027000
				1	-0.394021000	1.571040000	1.679694000
				1	-0.456685000	-1.559072000	0.905272000
				1	1.893299000	-1.844508000	-0.314719000
				1	-2.782140000	-1.724176000	0.147045000
				1	-2.609753000	-0.105361000	-0.739753000
				1	-3.341082000	0.176700000	1.621052000
				1	0.005321000	1.937309000	-1.129227000
				8	1.981289000	-0.994552000	0.137050000
				8	1.203632000	-0.153379000	-0.759715000
TS3c	**5.73E-04**	**9**	**2**	6	-0.840080000	1.411357000	-0.843355000
				6	0.178980000	0.601772000	-0.089357000
				6	1.054573000	-0.257950000	-0.750805000
				6	2.241602000	-0.896602000	-0.116022000
				8	0.628052000	1.128955000	1.088439000
				1	-1.619656000	1.765921000	-0.165667000
				1	-1.317499000	0.806899000	-1.613901000
				1	-0.358676000	2.277417000	-1.307412000
				1	0.785121000	-0.544013000	-1.761670000
				1	-1.761737000	-2.064843000	-0.231335000
				1	2.173017000	-1.990390000	-0.159497000
				1	2.339411000	-0.594875000	0.925773000
				1	3.165272000	-0.622803000	-0.641794000
				1	-0.145273000	1.382654000	1.607296000
				8	-2.020383000	-1.145681000	-0.077356000
				8	-0.991474000	-0.679203000	0.757097000
TS3d	**6.87E-04**	**9**	**2**	6	-1.061039000	1.276509000	-0.877013000
				6	-0.093099000	0.224735000	-0.439328000
				6	1.266035000	0.334915000	-0.498377000
				6	2.250039000	-0.737824000	-0.161913000
				8	0.238370000	1.057688000	1.567539000
				1	-1.826337000	1.420141000	-0.117911000
				1	-1.541960000	0.981575000	-1.816474000
				1	-0.535463000	2.218668000	-1.025516000
				1	1.650774000	1.294099000	-0.821040000
				1	-2.365233000	-1.575694000	-0.172532000
				1	2.770819000	-1.089321000	-1.060980000
				1	1.768833000	-1.599010000	0.301518000
				1	3.014668000	-0.349834000	0.517669000
				1	0.392713000	0.188928000	1.969120000

				8	-1.859837000	-1.019068000	0.436413000
				8	-0.566087000	-1.048566000	-0.243210000
TS3e	5.18E-04	9	2	6	1.174605000	1.211241000	0.865570000
				6	0.096208000	0.559574000	0.010916000
				6	-0.801622000	-0.392394000	0.722731000
				6	-2.094415000	-0.835699000	0.163782000
				8	-0.699514000	1.519161000	-0.657805000
				1	1.828010000	1.810329000	0.223321000
				1	1.781479000	0.441221000	1.341365000
				1	0.729061000	1.861478000	1.621439000
				1	-0.352672000	-0.966924000	1.523679000
				1	2.145623000	-1.727218000	-0.739580000
				1	-1.995937000	-1.843683000	-0.263045000
				1	-2.456725000	-0.156552000	-0.605554000
				1	-2.840501000	-0.917165000	0.963997000
				1	-0.107070000	2.072886000	-1.180117000
				8	1.455119000	-1.701518000	-0.061457000
				8	0.621905000	-0.296482000	-0.963676000
TS4a	7.81E-04	3	2	6	1.731117000	-1.084908000	-0.539806000
				6	0.744972000	-0.134883000	0.058659000
				6	-1.209859000	-1.288130000	0.140472000
				6	-2.334123000	-0.527026000	-0.032699000
				8	1.031187000	0.240289000	1.335020000
				1	2.727385000	-0.628464000	-0.569800000
				1	1.435201000	-1.353605000	-1.554036000
				1	1.785266000	-1.987802000	0.071015000
				1	-0.910414000	-1.597782000	1.135612000
				1	-0.856511000	-1.908647000	-0.675683000
				1	-2.776087000	-0.385870000	-1.013211000
				1	-1.271000000	1.326846000	-0.269106000
				1	-2.849044000	-0.077722000	0.810109000
				1	0.495016000	1.029175000	1.509889000
				8	-0.434056000	1.825607000	-0.164790000
				8	0.481312000	0.908298000	-0.820798000
TS4b	5.23E-04	3	2	6	1.790955000	-0.816975000	-0.385230000
				6	0.460724000	-0.202467000	0.049134000
				6	-0.754154000	-0.886303000	-0.549512000
				6	-1.961955000	-0.886834000	0.035278000
				8	0.316164000	-0.165950000	1.438322000
				1	2.613689000	-0.201221000	-0.015180000
				1	1.864735000	-0.877092000	-1.472506000
				1	1.872728000	-1.818361000	0.037078000
				1	-0.230416000	-2.858791000	-0.222479000
				1	-0.645400000	-1.176141000	-1.590103000
				1	-2.830719000	-1.288046000	-0.473896000
				1	-1.236462000	1.693407000	-0.744737000
				1	-2.080167000	-0.540486000	1.053897000
				1	0.949634000	0.477524000	1.776623000
				8	-0.564132000	1.946345000	-0.093867000
				8	0.561587000	1.137690000	-0.500294000
TS4c	4.04E-04	3	2	6	-0.388882000	1.250234000	-1.147357000
				6	0.038797000	0.471157000	0.090315000
				6	1.555189000	0.391858000	0.319953000
				6	1.845428000	-0.994694000	-0.175494000
				8	-0.605435000	0.915033000	1.243824000

1	**-1.454743000**	**1.105424000**	**-1.327155000**
1	**0.157357000**	**0.908421000**	**-2.029525000**
1	**-0.193162000**	**2.314071000**	**-0.993880000**
1	**1.746902000**	**0.488801000**	**1.388270000**
1	**2.100573000**	**1.171601000**	**-0.218946000**
1	**2.037184000**	**-1.171406000**	**-1.225754000**
1	**-1.918876000**	**-1.820642000**	**0.399113000**
1	**2.111005000**	**-1.787127000**	**0.510314000**
1	**-1.530750000**	**0.653822000**	**1.127195000**
8	**-1.871686000**	**-1.027202000**	**-0.150456000**
8	**-0.192714000**	**-0.959617000**	**-0.112635000**

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