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SUPPORTING INFORMATION FOR

Computational Kinetics by Variational Transition State Theory with Semiclassical Multidimensional Tunneling: Direct Dynamics Rate Constants for the Abstraction of H from CH_3OH by Triplet Oxygen Atoms

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Cartesian coordinates of the stationary points for the hydrogen abstraction reaction of H from CH_3OH by $O(^3P)$ optimized at M08-HX/MG3S level of theory. Absolute energies are in hartree.

Methanol
E=-115.724176

C	0.66052100	-0.02072400	0.00000000
H	1.08632400	0.98437700	-0.00000300
H	1.02372100	-0.54592900	0.89249500
H	1.02372000	-0.54593400	-0.89249200
O	-0.74325100	0.12184800	0.00000000
H	-1.15088000	-0.74295300	0.00000000

O(3P)
E=-75.055279

Transition state for reaction R1 TS(R1)
E=-190.770891

O	1.92373900	-0.20826800	-0.01307900
H	0.70013200	0.23256800	-0.01916700
C	-0.48717200	0.60998500	0.03608800
H	-0.54512700	1.11201300	1.00826100
H	-0.59164800	1.29772300	-0.80296400
O	-1.33614700	-0.45442200	-0.12054700
H	-1.34106300	-1.00069600	0.66635100

Transition structure for reaction R2 TS(R2)
E=-190.758348

C	1.25148800	0.19600200	0.00000000
O	0.00000000	0.80103800	0.00000000
H	1.97357600	1.02621100	0.00000000
H	1.42595300	-0.40238300	0.90117300
H	1.42595300	-0.40238300	-0.90117300
H	-0.87703700	0.04016600	0.00000000
O	-1.43217100	-0.98074100	0.00000000

Radical $CH_2^{\bullet}OH$
E=-115.059751

C	-0.67909800	0.02754400	-0.05291100
H	-1.24111200	-0.88335900	0.08295100
H	-1.11367100	1.00010500	0.13815800
O	0.66548400	-0.12540400	0.01855100
H	1.10549500	0.72122200	-0.05205200

Radical $CH_3O^{\bullet}$

E=-115.044809

C	0.57328800	0.00000900	-0.01257000
H	0.99993800	-0.90864000	-0.46069900
H	0.87301100	-0.00032000	1.05307100
H	0.99999700	0.90886700	-0.46021200
O	-0.78908400	0.00000500	-0.00709300

Radical $^{\bullet}OH$

E=-75.727156

O	0.00000000	0.00000000	0.10779100
H	0.00000000	0.00000000	-0.86233100

Geometries of methanol and transition states optimized at M08-SO/maug-cc-pVTZ level of theory used for the dynamics calculations.

Methanol

H	-1.155293000	-0.746481000	-0.000002000
O	-0.745193000	0.122674000	0.000000000
C	0.663249000	-0.020814000	-0.000001000
H	1.024010000	-0.548413000	0.894750000
H	1.089309000	0.986674000	0.000072000
H	1.024019000	-0.548291000	-0.894817000

Transition state for reaction R1 TS(R1)

H	-1.336893000	-1.004007000	0.670820000
O	-1.330433000	-0.456200000	-0.121775000
C	-0.491339000	0.615172000	0.036747000
H	-0.534569000	1.106852000	1.016689000
H	-0.585937000	1.301371000	-0.806858000
H	0.737649000	0.223760000	-0.019302000
O	1.913906000	-0.208676000	-0.013454000

Transition structure for reaction R2 TS(R2)

H	-0.881816000	0.052838000	0.000000000
O	0.000000000	0.803051000	0.000000000
C	1.256349000	0.190730000	0.000000000
H	1.424890000	-0.410102000	0.902888000
H	1.981025000	1.021271000	0.000000000
H	1.424890000	-0.410102000	-0.902888000
O	-1.435885000	-0.977837000	0.000000000