

SUPPORTING INFORMATION FOR:
Non-Hermitian Multiconfiguration Molecular Mechanics

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TABLE S I: Force Field Parameters.

	Morse parameters			angle bending parameters	
	H-H in H ₂	O-H in OH	O-H in H ₂ O	H-O-H	
r_e , Å	0.73789	0.96743	0.95308		
f , mdyn/Å	6.1	8.34	9.1		
D_e , kJ/mol	436.0 ^a	427.6 ^a	492.3		
\angle HOH, degree				106	
f , mdyn/rad				0.68	
c, q, p, s ^b				MM3 ^c	
	van der Waals parameters (atomic) ^d				
	atomic H	H in H ₂	H in H ₂ O	O in OH	O in H ₂ O
r_m , Å	1.32	1.20	1.32	1.62	1.82
ϵ , kcal/mol	0.016	0.016	0.008	0.059	0.059

^a D_e was set to be equal to D_{298}^0 of ref 1.

^bCubic, quartic, pentic, and sextic coefficients in the Taylor series.

^cRef 2.

^dCoefficients in the exp-6-12 van der Waals energy term (eq 40 of ref 3) are: $A = 18400$,² $B = 12.0$,² $C = 2.5$,² and $D = 0.05$.

Cartesian coordinates (in bohrs) of electronic structure Shepard points for PES1

*POINT 1

O -2.64166342E-17 5.97594033E-01 0.00000000E+00
H 1.79627053E+00 2.84614235E-01 0.00000000E+00
H -8.38336204E-01 -1.75642210E+00 0.00000000E+00
H -9.57934325E-01 -3.30894440E+00 0.00000000E+00

*POINT 2

O -5.04796719E-01 -2.00802156E-01 0.00000000E+00
H -8.88589877E-01 1.56861800E+00 0.00000000E+00
H 1.40037233E+00 -2.11474651E-01 0.00000000E+00
H 3.52659130E+00 2.49273901E-01 0.00000000E+00

*POINT 3

O -6.47245631E-01 -2.01804082E-01 0.00000000E+00
H -8.84522409E-01 1.61033175E+00 0.00000000E+00
H 2.37538419E+00 -2.77742059E-01 0.00000000E+00
H 3.68710327E+00 2.81842968E-01 0.00000000E+00

*POINT 4

O -5.79467613E-01 -1.83322215E-01 0.00000000E+00
H -9.08597331E-01 1.58844027E+00 0.00000000E+00
H 1.21494401E+00 -3.59938100E-01 0.00000000E+00
H 4.32939422E+00 2.38075555E-01 0.00000000E+00

*POINT 5

O -5.28278153E-01 -1.91548840E-01 0.00000000E+00
H -9.18064600E-01 1.56890048E+00 0.00000000E+00
H 1.27900659E+00 -2.98476969E-01 0.00000000E+00
H 3.86528324E+00 2.61967209E-01 0.00000000E+00

*POINT 6

O -5.35803333E-01 -2.05878260E-01 0.00000000E+00
H -8.86755661E-01 1.58020019E+00 0.00000000E+00
H 1.75872482E+00 -1.75508537E-01 0.00000000E+00
H 3.41445751E+00 2.42334430E-01 0.00000000E+00

*POINT 7

O	-5.47451827E-01	-2.06196975E-01	0.00000000E+00
H	-8.86700646E-01	1.58367801E+00	0.00000000E+00
H	1.84901194E+00	-1.75982794E-01	0.00000000E+00
H	3.41730333E+00	2.41880582E-01	0.00000000E+00

*POINT 8

O	-5.89494423E-01	-2.05090359E-01	0.00000000E+00
H	-8.84321715E-01	1.59650276E+00	0.00000000E+00
H	2.09488234E+00	-2.05326904E-01	0.00000000E+00
H	3.50539477E+00	2.49547010E-01	0.00000000E+00

*POINT 9

O	-7.03637423E-01	-1.98542389E-01	0.00000000E+00
H	-8.89559233E-01	1.62055818E+00	0.00000000E+00
H	2.64774200E+00	-3.66820059E-01	0.00000000E+00
H	3.87091661E+00	3.34600990E-01	0.00000000E+00

*POINT 10

O	-7.59736724E-01	-1.95963894E-01	0.00000000E+00
H	-8.94589401E-01	1.62735388E+00	0.00000000E+00
H	2.92655643E+00	-4.52107665E-01	0.00000000E+00
H	4.04592676E+00	3.92464937E-01	0.00000000E+00

*POINT 11

O	-5.17399156E-01	-2.03965968E-01	0.00000000E+00
H	-8.85127297E-01	1.57438325E+00	0.00000000E+00
H	1.57479529E+00	-1.87474342E-01	0.00000000E+00
H	3.44952525E+00	2.44818833E-01	0.00000000E+00

*POINT 12

O	-8.57185832E-17	7.10854686E-01	-1.75239210E-32
H	1.80261274E+00	3.98042498E-01	-2.64766933E-32
H	-8.57784042E-01	-1.87161235E+00	5.40685601E-32
H	-9.44828702E-01	-4.21326763E+00	1.12599501E-31

Cartesian coordinates (in bohrs) of electronic structure Shepard points for PES2

*POINT 1

O	-2.64166342E-17	5.97594033E-01	0.00000000E+00
H	1.79627053E+00	2.84614235E-01	0.00000000E+00
H	-8.38336204E-01	-1.75642210E+00	0.00000000E+00
H	-9.57934325E-01	-3.30894440E+00	0.00000000E+00

*POINT 2

O	-6.47245631E-01	-2.01804082E-01	0.00000000E+00
H	-8.84522409E-01	1.61033175E+00	0.00000000E+00
H	2.37538419E+00	-2.77742059E-01	0.00000000E+00
H	3.68710327E+00	2.81842968E-01	0.00000000E+00

*POINT 3

O	7.28108461E-18	6.48689260E-01	0.00000000E+00
H	1.79951655E+00	3.37009864E-01	0.00000000E+00
H	-9.08816840E-01	-2.03756415E+00	0.00000000E+00
H	-8.90699709E-01	-3.48895979E+00	0.00000000E+00

*POINT 4

O	9.15184852E-17	5.75406825E-01	0.00000000E+00
H	1.79220971E+00	2.62076457E-01	0.00000000E+00
H	-7.93921077E-01	-1.56659943E+00	0.00000000E+00
H	-9.98288636E-01	-3.29873162E+00	0.00000000E+00

*POINT 5

O	3.95559212E-17	6.91636642E-01	0.00000000E+00
H	1.80103794E+00	3.80948804E-01	0.00000000E+00
H	-9.93175609E-01	-2.25283339E+00	0.00000000E+00
H	-8.07862329E-01	-3.66120855E+00	0.00000000E+00

*POINT 6

O	4.92479821E-17	5.47043285E-01	0.00000000E+00
H	1.78683955E+00	2.36593778E-01	0.00000000E+00
H	-7.25958839E-01	-1.29211003E+00	0.00000000E+00
H	-1.06088071E+00	-3.32083002E+00	0.00000000E+00

*POINT 7

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O  9.04491412E-17  7.05473623E-01  0.00000000E+00
H  1.80119621E+00  3.94602240E-01  0.00000000E+00
H -1.01897906E+00 -2.32152059E+00  0.00000000E+00
H -7.82217155E-01 -3.71687064E+00  0.00000000E+00
*POINT 8
O -2.20087429E-17  6.29601048E-01  0.00000000E+00
H  1.79846531E+00  3.16859254E-01  0.00000000E+00
H -8.84564099E-01 -1.93845153E+00  0.00000000E+00
H -9.13901208E-01 -3.41521610E+00  0.00000000E+00
*POINT 9
O  5.06715287E-18  5.45296703E-01  0.00000000E+00
H  1.78670892E+00  2.40586270E-01  0.00000000E+00
H -7.23082141E-01 -1.27316174E+00  0.00000000E+00
H -1.06362678E+00 -3.32979815E+00  0.00000000E+00

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Cartesian coordinates (in Angstroms) of the molecular mechanics
Shepard points (the same geometries for PES1 and PES2)

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O    1.474421    1.284490   -1.151629
H    2.417010    1.105645   -1.027283
H    2.194150   -.809362    .599616
H    2.202611   -1.199975   -.026349

O    -.134850    .000000    1.022265
H    .065505    .000000    .090482
H    .704788    .000000    1.473231
H    2.701698    .000000   -.289150

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TABLE S II: Comparison of the Rate Coefficients ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) Calculated by Direct Dynamics and Using MCMM Surfaces for $\text{OH} + \text{H}_2 \rightarrow \text{HOH} + \text{H}$ and $\text{HOH} + \text{H} \rightarrow \text{OH} + \text{H}_2$

T	CVT	CVT/ZCT	CVT/SCT	CVT/LCT	CVT/ μ OMT
$\text{OH} + \text{H}_2 \rightarrow \text{HOH} + \text{H}$					
Direct Dynamics					
250	4.35E-16	2.19E-15	4.01E-15	2.37E-15	4.01E-15
300	2.64E-15	7.65E-15	1.15E-14	7.95E-15	1.15E-14
400	2.55E-14	4.48E-14	5.57E-14	4.54E-14	5.57E-14
600	2.69E-13	3.39E-13	3.71E-13	3.40E-13	3.71E-13
1000	2.27E-12	2.40E-12	2.48E-12	2.40E-12	2.48E-12
PES1					
250	3.94E-16	1.89E-15	4.11E-15	1.92E-15	4.11E-15
300	2.42E-15	6.64E-15	1.11E-14	6.78E-15	1.11E-14
400	2.38E-14	4.02E-14	5.29E-14	4.07E-14	5.29E-14
600	2.54E-13	3.08E-13	3.46E-13	3.09E-13	3.46E-13
1000	2.16E-12	2.29E-12	2.38E-12	2.29E-12	2.38E-12
PES2					
250	4.35E-16	2.24E-15	4.66E-15	2.25E-15	4.66E-15
300	2.64E-15	7.69E-15	1.27E-14	7.81E-15	1.27E-14
400	2.54E-14	4.31E-14	5.67E-14	4.34E-14	5.67E-14
600	2.63E-13	3.26E-13	3.68E-13	3.27E-13	3.68E-13
1000	2.21E-12	2.35E-12	2.46E-12	2.36E-12	2.47E-12
$\text{HOH} + \text{H} \rightarrow \text{OH} + \text{H}_2$					
Direct Dynamics					
250	3.46E-26	1.75E-25	3.19E-25	1.89E-25	3.19E-25
300	1.24E-23	3.59E-23	5.40E-23	3.74E-23	5.40E-23
400	2.03E-20	3.56E-20	4.43E-20	3.61E-20	4.43E-20
600	3.81E-17	4.79E-17	5.26E-17	4.81E-17	5.26E-17
1000	2.09E-14	2.21E-14	2.29E-14	2.22E-14	2.29E-14
PES1					
250	3.16E-26	1.51E-25	3.29E-25	1.54E-25	3.29E-25
300	1.15E-23	3.14E-23	5.27E-23	3.21E-23	5.27E-23
400	1.91E-20	3.23E-20	4.24E-20	3.26E-20	4.24E-20
600	3.64E-17	4.41E-17	4.95E-17	4.43E-17	4.95E-17
1000	2.02E-14	2.14E-14	2.22E-14	2.14E-14	2.22E-14
PES2					
250	3.48E-26	1.79E-25	3.73E-25	1.80E-25	3.73E-25
300	1.251E-23	3.64E-23	6.00E-23	3.70E-23	6.00E-23
400	2.04E-20	3.46E-20	4.55E-20	3.49E-20	4.55E-20
600	3.77E-17	4.67E-17	5.27E-17	4.68E-17	5.27E-17
1000	2.06E-14	2.20E-14	2.30E-14	2.20E-14	2.30E-14

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