Supporting Information for
"Improved Interpolated Correction Schemes for Dual-Level Direct Dynamics Calculation"

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Table S1: Calculated Stationary Point Geometry (in angstroms and degrees) of R1

	MNDO	HF/3-21+G*	HF/6-31+G**	MP2/3-21+G*	MP2/6-31G**
H₂S (C₂ᵥ)					
r(S–H)	1.299	1.327	1.327	1.338	1.330
∠H–S–H	98.0	94.4	94.4	93.5	92.9
HS					
r(S–H)	1.294	1.330	1.331	1.342	1.335
H₂					
r(H–H)	0.663	0.735	0.733	0.741	0.734
Transition State H3–S···H2···H1					
r(H1–H2)	1.054	1.059	1.058	1.038	1.062
r(S–H2)	1.366	1.485	1.479	1.478	1.477
r(S–H3)	1.298	1.329	1.329	1.340	1.333
∠(H1–H2–S)	177.9	176.7	175.7	176.7	175.9
∠(H2–S–H3)	98.4	92.0	92.2	91.4	91.0
Dihedral Angle	0.0	0.0	0.0	0.0	0.0

Table S2: Calculated Vibrational Frequencies (in cm^{-1}) of the Stationary Points of R1

	MNDO	HF/3-21+G*	HF/6-31+G**	MP2/3-21+G*	MP2/6-31G**
H$_2$S					
	3037.5	2904.5	2909.0	2801.8	2858.7
	3008.7	2899.9	2896.1	2781.7	2832.5
	1234.6	1372.3	1337.7	1286.0	1266.2
H$_2$					
	4293.1	4657.5	4635.5	4551.3	4612.8
HS					
	3038.2	2877.1	2881.1	2761.0	2815.7
Transition State					
	3025.4	2886.8	2890.3	2775.2	2830.1
	1755.5	1290.0	1283.5	1300.4	1400.8
	1134.7	1219.0	1211.9	1223.2	1198.4
	364.0	800.2	723.4	766.1	653.9
	330.0	297.6	561.0	594.8	548.9
	1401.9 *i*	2288.7 *i*	2262.6 *i*	2125.5 *i*	1846.7 *i*

Table S3: Calculated Rate Constants in cm^3 molecule^{-1} s^{-1} of R1 at MNDO Level

T(K)	TST	CVT	CVT/SCT	CVT/LCT
200	1.48(−15)	5.78(−16)	6.41(−15)	3.60(−15)
250	1.27(−14)	6.31(−15)	2.96(−14)	1.92(−14)
300	5.53(−14)	3.22(−14)	9.39(−14)	6.79(−14)
400	3.72(−13)	2.64(−13)	4.77(−13)	3.92(−13)
500	1.25(−12)	9.93(−13)	1.43(−12)	1.25(−12)
600	2.96(−12)	2.51(−12)	3.18(−12)	2.90(−12)
800	9.59(−12)	8.77(−12)	9.69(−12)	9.19(−12)
1000	2.13(−11)	2.01(−11)	2.09(−11)	2.02(−11)

Table S4: Calculated Rate Constants in cm^3 molecule^{-1} s^{-1} of R1 at HF/3-21+G* Level

T(K)	TST	CVT	CVT/SCT	CVT/LCT
200	1.61(−23)	1.61(−23)	4.80(−18)	4.38(−18)
250	4.85(−21)	4.85(−21)	2.05(−17)	1.98(−17)
300	2.20(−19)	2.20(−19)	8.81(−17)	6.47(−17)
400	2.67(−17)	2.67(−17)	7.93(−16)	4.62(−16)
500	4.98(−16)	4.98(−16)	4.41(−15)	2.52(−15)
600	3.67(−15)	3.67(−15)	1.67(−14)	1.04(−14)
800	4.90(−14)	4.90(−14)	1.15(−13)	8.45(−14)
1000	2.55(−13)	2.55(−13)	4.38(−13)	3.57(−13)

Table S5: Calculated Rate Constants in cm^3 $molecule^{-1}$ s^{-1} of R1 at MP2/3-21+G* Level

T(K)	TST	CVT	CVT/SCT	CVT/LCT
200	3.30(−22)	3.29(−22)	4.91(−18)	1.81(−17)
250	5.41(−20)	5.40(−20)	2.77(−17)	7.95(−17)
300	1.63(−18)	1.63(−18)	1.29(−16)	2.56(−16)
400	1.19(−16)	1.19(−16)	1.41(−15)	1.66(−15)
500	1.64(−15)	1.64(−15)	7.96(−15)	7.58(−15)
600	9.87(−15)	9.87(−15)	2.94(−14)	2.63(−14)
800	1.02(−13)	1.02(−13)	1.87(−13)	1.69(−13)
1000	4.53(−13)	4.52(−13)	6.66(−13)	6.15(−13)

Table S6: Calculated Rate Constants in cm^3 $molecule^{-1}$ s^{-1} of R1 at HF/6-31+G** Level

T(K)	TST	CVT	CVT/SCT	CVT/LCT
200	1.19(−23)	1.19(−23)	2.31(−18)	2.17(−18)
250	3.85(−21)	3.83(−21)	1.09(−17)	1.08(−17)
300	1.83(−19)	1.82(−19)	4.92(−17)	3.90(−17)
400	2.37(−17)	2.36(−17)	5.71(−16)	3.33(−16)
500	4.63(−16)	4.62(−16)	3.56(−15)	2.07(−15)
600	3.52(−15)	3.51(−15)	1.45(−14)	9.22(−15)
800	4.90(−14)	4.90(−14)	1.09(−13)	8.12(−14)
1000	2.61(−13)	2.61(−13)	4.34(−13)	3.57(−13)

Table S7: Estimated $s_{1/2}$ (in bohrs) of R1 by Different Intermediate-Level Calculation

Intermediate-Level	$s_{1/2}$
MP2/6-31+G**//MNDO	−0.714
MP2/6-31+G**//HF/3-21+G*	−0.635
MP2/6-31+G**//MP2/3-21+G*	−0.640
MP2/6-31+G**//HF/6-31+G**	−0.641

Table S8: Range Parameters Used in the Dual-Level[a] Calculation of R1

	L_1			L_2
Low Level	SECKART	SIL-1	SIL-2	SIL-3
MNDO	0.580	0.284(0.228)[b]	0.327(0.260)	
HF/3-21+G*	0.350	0.280	0.288	0.200
HF/6-31+G**	0.370	0.335	0.345	0.265
MP2/3-21+G*	0.370	0.157	0.167	

[a]The high level is MP2/6-31+G**.

[b]Numbers in parentheses are obtained using the MP2/6-31+G**//HF/3-21+G* intermediate level. All other values are obtained using the (high level)//(low level) as the intermediate level.

Table S9: Calculated Reactant and Product Geometry (in degrees and angstroms) of R2

	MP2/3-21+G	MP2/6-31G**	MP2/cc-pVDZ
CH_4 (T_d)			
r(C–H)	1.094	1.085	1.100
OH			
r(O–H)	1.007	0.972	0.975
CH_3 (D_{3h})			
r(C–H)	1.081	1.074	1.090
$\angle$(H–C–H)	120.0	120.0	120.0
H_2O (C_{2v})			
r(O–H)	0.990	0.961	0.965
$\angle$(H–O–H)	109.4	103.8	101.9

Table S10: Cartesian Coordinates (in angstroms) of the Transition State Geometry of R2 Calculated at MP2/3-21+G level

Atom	X	Y	Z
C	1.225182	−0.013285	0.000002
H	1.486225	−0.551664	−0.911542
H	−0.014352	0.102779	0.000042
H	1.563426	1.024126	−0.001512
H	1.486337	−0.549099	0.913025
O	−1.293004	0.114519	0.000000
H	−1.528693	−0.862584	−0.000025

Table S11: Cartesian Coordinates (in angstroms) of the Transition State Geometry of R2 Calculated at MP2/6-31G** level

Atom	X	Y	Z
C	−1.190752	0.007463	−0.000019
H	−1.556390	−0.533635	−0.864595
H	0.001628	−0.169381	0.008513
H	−1.555388	−0.404186	0.933539
H	−1.377860	1.072100	−0.077209
O	1.281620	−0.108405	−0.000036
H	1.379562	0.857564	0.000154

Table S12: Cartesian Coordinates (in angstroms) of the Transition State Geometry of R2 Calculated at MP2/cc-pVDZ level

Atom	X	Y	Z
C	-1.191343	0.006112	0.000003
H	-1.571703	-0.469322	0.913329
H	0.006179	-0.190966	0.000060
H	-1.363390	1.090274	-0.001877
H	-1.572005	-0.472501	-0.911536
O	1.288758	-0.107423	0.000000
H	1.338916	0.865226	0.000002

Table S13: Calculated Vibrational Frequencies (in cm^{-1}) of the Reactants and Products of R2

	MP2/3-21+G	MP2/6-31G**	MP2/cc-pVDZ
CH$_4$			
	3171.8	3279.1	3232.8
	3171.8	3279.1	3232.8
	3171.3	3279.1	3232.8
	3065.9	3133.1	3081.5
	1648.9	1624.1	1565.4
	1648.9	1624.1	1565.4
	1439.0	1404.5	1338.5
	1439.0	1404.5	1338.5
	1438.9	1404.5	1338.5
OH			
	3375.5	3841.9	3790.9
CH$_3$			
	3341.7	3438.0	3383.8
	3341.7	3438.0	3383.8
	3160.7	3240.6	3179.4
	1490.2	1488.5	1427.7
	1490.2	1488.5	1427.7
	512.2	389.5	383.0
H$_2$O			
	3656.8	4030.6	3970.8
	3484.3	3892.2	3851.5
	1612.5	1682.1	1677.9

Table S14: Calculated Vibrational Frequencies (in cm^{-1}) of the Transition State of R2

MP2/3-21+G	MP2/6-31G**	MP2/cc-PVDZ
3403.5	3843.1	3799.6
3235.0	3318.9	3270.6
3232.2	3313.0	3266.1
3105.5	3173.7	3122.1
1559.3	1542.2	1508.5
1532.9	1518.7	1465.1
1455.3	1462.6	1419.4
1348.3	1325.3	1267.5
1299.5	1201.3	1173.9
909.9	939.2	922.3
610.6	744.5	765.0
423.7	353.2	377.3
384.3	280.2	295.0
66.7	32.4	32.2
2284.7 i	2061.2 i	1933.6 i

Table S15: Calculated Rate Constants in cm^3 molecule^{-1} s^{-1} of R2 at MP2/3-21+G Level

T(K)	TST	CVT	CVT/SCT	CVT/LCT
200	2.50(−24)	2.25(−24)	3.79(−22)	3.39(−21)
250	8.77(−22)	8.36(−22)	1.63(−20)	5.35(−20)
300	4.55(−20)	4.38(−20)	3.15(−19)	5.65(−19)
400	7.04(−18)	6.85(−18)	1.97(−17)	2.17(−17)
500	1.63(−16)	1.60(−16)	3.07(−16)	3.01(−16)
600	1.45(−15)	1.42(−15)	2.31(−15)	2.21(−15)
800	2.68(−14)	2.40(−14)	3.15(−14)	3.02(−14)
1000	1.80(−13)	1.48(−13)	1.76(−13)	1.70(−13)

Table S16: Calculated Rate Constants in cm^3 molecule^{-1} s^{-1} of R2 at MP2/6-31G** Level

T(K)	TST	CVT	CVT/SCT	CVT/LCT
200	1.99(−22)	8.09(−24)	1.62(−21)	3.61(−21)
250	3.59(−20)	2.47(−21)	6.32(−20)	6.96(−20)
300	1.20(−18)	1.17(−19)	1.10(−18)	8.86(−19)
400	1.07(−16)	1.57(−17)	5.68(−17)	4.23(−17)
500	1.78(−15)	3.26(−16)	7.53(−16)	5.92(−16)
600	1.27(−14)	2.64(−15)	4.75(−15)	3.94(−15)
800	1.78(−13)	4.12(−14)	5.74(−14)	5.11(−14)
1000	1.01(−12)	2.42(−13)	2.98(−13)	2.76(−13)

Table S17: Estimated $s_{1/2}$ (in bohrs) of R2 by Different Intermediate-Level Calculation

Intermediate-Level	$s_{1/2}$
MP2/cc-pVDZ//MP2/3-21+G	−1.155
MP2/cc-pVDZ//MP2/6-31G**	−1.140

Table S18: Range Parameters Used in the Dual-Level[a] Calculation of R2

	L_1			L_2
Low Level	SECKART	SIL-1	SIL-2	SIL-3
MP2/3-21+G	0.680	0.470	0.330	
MP2/6-31G**	0.600	0.610	0.555	1.700

[a]The high level is MP2/cc-pVDZ.