

Effect of Formic Acid on $O_2+OH\cdot CHO H\rightarrow HCOOH+HO_2$ Reaction Under Tropospheric Condition: Kinetics of Cis and Trans Isomers

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Table S1: Redundant internal coordinates of reactants, complexes, products and transition states obtained using M06-2X /6-311++G(3df,3pd) for $OH\cdot CHO H + O_2 \rightarrow HCOOH + HO_2$

Cis- $OH\cdot CHO H$

Charge = 0 Multiplicity = 2, Electronic State -2A, Point Group: C1

Redundant internal coordinates found in file.

C,0,0.0131837108,0.5259092875,-0.1524580546

H,0,-0.0850688989,1.5116169475,0.3095320457

O,0,1.1649715044,-0.1472021743,0.1012571593

O,0,-1.0332095458,-0.3240267851,0.0110439243

H,0,-1.8477253978,0.1413930006,-0.1874420225

H,0,1.9082024372,0.4434870738,-0.0334353921

O_2

Charge = 0 Multiplicity = 3, Electronic State -3SGG, Point Group: $D_{\infty h}$

Redundant internal coordinates found in file.

O,0,-1.9006779975,-0.42031795,-0.00550226

O,0,-3.0883555625,-0.42031795,-0.00550226

$OH\cdot C(OO)HOH$ (c-Int)

Charge = 0 Multiplicity = 2, Electronic State -2A, Point Group: C1

Redundant internal coordinates found in file.

C,0,0.382923372,-0.0203467387,0.5407266659

H,0,0.7736989899,-0.0844871594,1.5547871072

O,0,-0.733657329,-0.9847235065,0.5594461135

O,0,-1.4751781351,-0.8391393822,-0.4893020727

H,0,-0.4195627958,1.2397557594,-0.5983263245

O,0,-0.0577999396,1.226881807,0.2976728594

O,0,1.2680183035,-0.4120186774,-0.4339388189

H,0,1.5115287541,-1.3335997622,-0.30584127

c-TS

Charge = 0 Multiplicity = 2, Electronic State: 2-A, Point Group: C1

Redundant internal coordinates found in file.

C,0,0.7171794599,0.1614406432,0.408026634

H,0,0.8386252506,-0.057227301,1.4698110453

O,0,-0.8614478899,-0.8522869563,0.2214291907

O,0,-1.6568828432,0.0036451038,-0.2744658302

H,0,-0.862541897,0.9420405177,-0.2566887159

O,0,0.2436473918,1.2643342566,0.0245588865

O,0,1.5651297723,-0.4665000626,-0.4126483846

H,0,1.9208977555,-1.2557932014,0.0064091742

OHCH(OOH)O• (c-Post Int)

Charge = 0 Multiplicity = 2, Electronic State: 2-A, Point Group: C1

Redundant internal coordinates found in file.

C,0,1.5587539605,0.4268651466,0.4176426921

H,0,1.5052970091,0.0577229256,1.4481982834

O,0,-0.7944859821,-0.8853535486,0.26511722

O,0,-1.4204890687,0.1478393386,-0.2077475373

H,0,-0.7448610324,0.864812205,-0.24108575
O,0,0.9612827189,1.3885815413,0.0292148173
O,0,2.3689189487,-0.2606737205,-0.3808775284
H,0,2.734420346,-1.022652288,0.0794486529

c-HCOOH

Charge = 0 Multiplicity = 1, Electronic State:1-A, Point Group: Cs

Redundant internal coordinates found in file.

C,0,-0.9824887855,-0.3317804999,-0.2116485219
H,0,-2.0307268652,-0.1008107908,0.0316098649
O,0,-0.4072661868,-1.2860450481,0.1910368641
O,0,-0.401959632,0.5735250665,-1.0158240323
H,0,-1.0228401505,1.2736854623,-1.2367298248

HO₂

Charge = 0 Multiplicity = 2 Electronic State:2-A, Point Group: Cs

Redundant internal coordinates found in file.

O,0,-1.5852942928,0.3567774158,0.
H,0,-1.8786597338,1.2835533288,0.
O,0,-0.2820756934,0.3929236454,0.

trans-OH•CHOH

Charge = 0 Multiplicity = 2, Electronic State:2-A, Point Group: C1

Redundant internal coordinates found in file.

C,0,-0.9537673537,0.8221184157,-0.0835471081
H,0,-0.4508599698,1.1013201204,-1.0053485136
O,0,-1.9403177597,-0.0761672221,-0.2916015115
H,0,-2.2544829149,-0.3876337743,0.5632407494
O,0,-0.1629206711,0.4771829843,0.9828741634
H,0,0.4030896693,1.218251406,1.2091482305

OH•C(OO)HOH (t-Int)

Charge = 0 Multiplicity = 2, Electronic State:2-A, Point Group: C1

Redundant internal coordinates found in file.

C,0,0.377217927,-0.1040307517,0.2695313476
H,0,0.3397520634,-0.1881834516,1.3555610804
O,0,-0.7156141446,-0.9814045138,-0.2203361714
O,0,-1.86262429,-0.4361196668,0.009060054
H,0,-0.7502477184,1.3932698795,-0.0250961005
O,0,0.1686449033,1.1564432053,-0.2057536152
O,0,1.5330627686,-0.6210558518,-0.1903076952
H,0,1.6403407108,-0.3551412091,-1.1113683798

t-TS

Charge = 0 Multiplicity = 2, Electronic State:2-A, Point Group: C1

Redundant internal coordinates found in file.

C,0,0.7093120036,0.1043117412,0.441125853
H,0,0.7773131555,-0.1318746316,1.4997673457
O,0,-0.8905260204,-0.8430977321,0.1771869537
O,0,-1.6658226083,0.059538186,-0.2712004145
H,0,-0.8425547306,0.9649416463,-0.2192964129
O,0,0.2894959126,1.2302053212,0.031218307
O,0,1.5973709576,-0.5823105845,-0.2712624954
H,0,1.61348133,-0.2193529465,-1.1662311368

OHCH(OOH)O• (t-Post Int).

Charge = 0 Multiplicity = 2, Electronic State:2-A, Point Group: Cs

Redundant internal coordinates found in file.

C,0,0.6569329937,-0.1679824076,0.051979555
H,0,0.2701431141,-0.8573245853,0.8044968434
O,0,-2.2161211005,-0.7904200878,0.9187548034
O,0,-2.6113502446,0.0800680644,0.0340507945
H,0,-1.7747633545,0.4071784473,-0.3715410149
O,0,-0.034813681,0.5357039799,-0.6355962168

O,0,1.9777900251,-0.1945625009,-0.0180913435

H,0,2.2634099876,0.43253215,-0.697746921

t-HCOOH

Charge = 0 Multiplicity = 1, Electronic State:1-A, Point Group: Cs

Redundant internal coordinates found in file.

C,0,-0.9679043176,-0.3299238169,-0.1731074849

H,0,-2.0020741395,-0.0902387101,0.0940844883

O,0,-0.4072866085,-1.3437756611,0.1043365453

O,0,-0.423828928,0.6807961879,-0.8567846863

H,0,0.4855081744,0.4340688913,-1.0745379901

Table S2: Redundant internal coordinates of reactants, complexes, products and transition states obtained using M06-2X/6-311++G(3df,3pd) for OH•CHOH + O2+ (FA).

c-Int-FA

Charge = 0 Multiplicity = 2, Electronic State:2-A, Point Group: C1

Redundant internal coordinates found in file.

C,0,1.5308876819,0.0928772455,0.8342233191

H,0,2.406663785,0.2658615887,1.4575653079

O,0,2.1242090397,0.2479057806,-0.5307139311

O,0,1.2551756859,0.0701737797,-1.4638552078

H,0,0.154565424,-1.2164855428,0.6749090298

O,0,1.0598029646,-1.1452296245,1.0194493143

O,0,0.5363394936,1.026406944,0.9700217729

H,0,0.9045900713,1.9141787603,0.9357862347

C,0,-2.1911653378,0.1064191333,-0.2182545396

H,0,-1.987937619,1.110269987,-0.6162134403

O,0,-3.1204153885,-0.161467751,0.4674488695

O,0,-1.279325301,-0.8102125766,-0.5893840178

H,0,-0.5541794997,-0.3930427242,-1.0860187117

c-TS-FA

Charge = 0 Multiplicity = 2, Electronic State:2-A, Point Group: C1

Redundant internal coordinates found in file.

C,0,1.3475375429,0.0183232009,0.8250885787

H,0,1.7476819341,-0.6926567053,1.5477363173

O,0,2.8722607036,0.1280793572,-0.1761200176

O,0,2.4737380408,-0.1901256584,-1.33855202

H,0,1.3291838708,-0.3943963052,-1.0291370715

O,0,0.5577660583,-0.3796005849,-0.0921033116

O,0,1.1696547502,1.2653497208,1.2615368844

H,0,1.7063993565,1.4461577191,2.0395673362

C,0,-2.7622176612,-0.239567355,-0.2577400446

H,0,-2.1887962979,-1.1798146468,-0.2444419787
O,0,-3.9510771605,-0.1991713893,-0.2699469678
O,0,-1.9935994578,0.8495789582,-0.2584474084
H,0,-1.0611006298,0.5846772388,-0.2371492464

c-PostInt-FA

Charge = 0 Multiplicity = 2, Electronic State:2-A, Point Group: C1

Redundant internal coordinates found in file.

C,0,1.215284258,0.8574388922,0.749364782
H,0,2.0323345499,0.9259345435,1.4722161962
O,0,3.095162131,-0.635097228,-0.3917873753
O,0,2.3755671585,-1.7122461948,-0.4567095825
H,0,1.5103046216,-1.4735905529,-0.0563504363
O,0,0.4758969288,-0.0920776157,0.6835297873
O,0,1.0522572628,1.9006990988,-0.040759564
H,0,1.729952396,2.5682728793,0.109673305
C,0,-2.8513037138,-0.3242996301,0.1366251309
H,0,-2.389347652,-0.623521056,1.0909991075
O,0,-4.0212957994,-0.3805678454,-0.0686168465
O,0,-1.9704134155,0.1062684678,-0.7668504042
H,0,-1.0782657258,0.0777392414,-0.3883091002

t-Int1-FA

Charge = 0 Multiplicity = 2, Electronic State:2-A, Point Group: C1

Redundant internal coordinates found in file.

C,0,-0.9400806437,0.1623396896,0.0443325651
H,0,-0.3239660957,-0.6178119825,0.4870162439
O,0,-1.8397775136,-0.5055925197,-0.9140723446
O,0,-2.7578008965,-1.1547341079,-0.2790738749
H,0,-2.3419301395,0.293933041,1.3174897274
O,0,-1.6866907462,0.8845962944,0.9256731651

O,0,-0.1538116444,0.9928397328,-0.6958133416
H,0,-0.6580289578,1.7885545992,-0.90538056
C,0,2.8175727208,-0.3746363915,0.2543829723
H,0,3.8798216287,-0.5987544861,0.3947260289
O,0,1.9301020019,-0.991055613,0.7713826353
O,0,2.6575300885,0.6592862209,-0.5564132644
H,0,1.7019361974,0.8308065229,-0.6556779523

t-TS₁-FA

Charge = 0 Multiplicity = 2, Electronic State:2-A, Point Group: C1

Redundant internal coordinates found in file.

C,0,-0.8641460215,0.6105041532,0.6557113865
H,0,-0.2829386772,0.1808626741,1.4642778193
O,0,-0.7238001046,-0.867320889,-0.4607147033
O,0,-1.9415816033,-1.1313472434,-0.7109500158
H,0,-2.4075820783,-0.2439432407,-0.027847345
O,0,-2.1276293501,0.6947579526,0.6705407456
O,0,-0.155098703,1.538930645,-0.0199429724
H,0,-0.7666453195,2.0195434817,-0.5934509398
C,0,2.5110594526,-0.6015058445,0.0237158733
H,0,3.3566318437,-1.2479426378,-0.2319182729
O,0,1.8824460142,-0.6885207422,1.0384742779
O,0,2.286666222,0.283297288,-0.9377944139
H,0,1.5174943251,0.8224554031,-0.6815294395

t-PostInt1-FA

Charge = 0 Multiplicity = 2, Electronic State:2-A, Point Group: C1

Redundant internal coordinates found in file.

C,0,-0.6686049133,-0.3719391538,-0.8031948081
H,0,0.1252239369,-0.6754965561,-1.4879325454
O,0,-3.7235137833,1.3463711319,1.6962965905

O,0,-2.8192838147,0.4993922261,1.2899210299
H,0,-3.0130667429,0.2497012294,0.361594247
O,0,-1.8425196858,-0.3945020891,-1.0415167197
O,0,-0.1500222829,0.0367286366,0.3622773828
H,0,-0.8627534977,0.3083388249,0.9669963966
C,0,3.1220053358,-0.5324134595,-0.455549686
H,0,4.2114893627,-0.6322795772,-0.4785499749
O,0,2.402857336,-0.8244552779,-1.3678482009
O,0,2.7162814527,-0.0489726497,0.7089551477
H,0,1.7450862966,0.0221247145,0.6900881404

t-Int2-FA

Charge = 0 Multiplicity = 2, Electronic State:2-A, Point Group: C1

Redundant internal coordinates found in file.

C,0,1.2333323595,0.5150778446,0.5161223192
H,0,2.1342294699,0.7384492282,1.0863170121
O,0,1.7102176889,0.1285878627,-0.8333160629
O,0,2.3078101643,-1.0146425309,-0.7905671306
H,0,1.1097795729,-1.3502111721,0.9220902469
O,0,0.5450129811,-0.5728438286,1.0352514941
O,0,0.4661451997,1.5931582288,0.3911402215
H,0,-0.3665840416,1.3693134841,-0.0796635264
C,0,-2.5271232022,-0.095782184,-0.4254880629
H,0,-3.5438389326,-0.2873569566,-0.779072475
O,0,-1.8836036992,0.8605208414,-0.7760121759
O,0,-2.1206877726,-1.025173996,0.4078903875
H,0,-1.195575788,-0.8447648217,0.6821097524

t-TS₂-FA

Charge = 0 Multiplicity = 2, Electronic State:2-A, Point Group: C1

Redundant internal coordinates found in file.

C,0,1.1152795622,0.5934038599,0.7235016354
H,0,1.9108158438,0.9069229579,1.3937870455
O,0,2.2592916606,0.0354233298,-0.6065720894
O,0,2.0188644635,-1.2105119017,-0.7110030457
H,0,1.1585039584,-1.2270618254,0.1640937549
O,0,0.5416828388,-0.5540033248,0.9217162235
O,0,0.4545942408,1.5944625186,0.2074105035
H,0,-0.3727426155,1.2850640382,-0.2411115924
C,0,-2.5248685181,-0.1146990192,-0.3451683109
H,0,-3.5647391916,-0.2977796808,-0.6286995226
O,0,-1.8735790584,0.784775374,-0.8204978845
O,0,-2.1033986343,-0.9730895592,0.5474761377
H,0,-1.15059055,-0.8085747673,0.751869145

t-PostInt2-FA

Charge = 0 Multiplicity = 2, Electronic State:2-A, Point Group: C1

Redundant internal coordinates found in file.

C,0,0.8645940024,0.7797737981,0.4270217476
H,0,1.9233188676,1.0021288847,0.567186108
O,0,3.477295339,-0.8148564812,-0.0234410942
O,0,2.732945295,-1.8035726953,-0.4311933203
H,0,1.8139662201,-1.4599775629,-0.3535035372
O,0,0.5004396686,-0.3093650288,0.002569367
O,0,0.0751558584,1.7510967148,0.7449948524
H,0,-0.8861738887,1.5050888775,0.6013377457
C,0,-2.8210805577,0.0156542856,-0.0572484618

H,0,-3.8841935457,-0.1975427894,-0.1942596601
O,0,-2.430006545,1.0829242954,0.3605532978
O,0,-2.0671119362,-0.9939541602,-0.3913724327
H,0,-1.1113837779,-0.7678111384,-0.2553906122

Table S3: Rotational-Vibrational parameters of reactants, complexes and transition states obtained using M06-2X/6-311++G(3df,3pd) for OH•CHOH + O₂.

	cis- CHOHOH	trans- CHOHOH	c-Int	c-TS	c-Post	t-Int	t-TS	t-Post
cm ⁻¹	248.57	298.39	132.13	914.04 <i>i</i>	36.83	132.84	947.99 <i>i</i>	79.43
cm ⁻¹	381	368.08	308.28	146.58	88.96	317.97	149.12	92.47
cm ⁻¹	547.4	553.33	332.78	315.91	191.27	375.70	306.16	116.71
cm ⁻¹	951.93	956.68	441.19	468.32	223.80	430.80	484.03	173.48
cm ⁻¹	1097.35	1092	488.24	606.52	289.71	497.01	597.11	225.83
cm ⁻¹	1133.16	1165.53	573.45	622.75	539.77	597.06	643.16	665.34
cm ⁻¹	1248.19	1220.29	786.32	722.79	571.66	648.89	716.68	670.69
cm ⁻¹	1357.65	1373.81	831.30	777.01	687.26	889.85	789.89	700.15
cm ⁻¹	1439.75	1426.02	1098.71	1070.35	1052.78	1083.09	1094.32	1094.22
cm ⁻¹	3050.1	3136.7	1196.96	1152.55	1178.63	1219.57	1160.75	1192.67
cm ⁻¹	3930.03	3880.88	1238.61	1177.55	1305.73	1252.36	1177.96	1303.22
cm ⁻¹	3930.4	3923.65	1261.06	1287.00	1314.10	1310.37	1343.85	1345.58
A(GHZ)	62.41178	57.23206	1382.31	1399.35	1441.96	1363.68	1376.82	1406.65
B(GHZ)	10.86984	11.02236	1417.91	1402.02	1541.93	1408.43	1395.97	1564.13
C(GHZ)	9.3841	9.43967	1471.17	1682.12	1864.36	1485.60	1640	1825.47
2D(GHZ)	10.09968641	10.20036	3155.31	1945.44	3095.36	3154.38	1941	3172.26
			3823.61	3134.52	3468.61	3828.03	3185	3431.19
			3894.80	3891.11	3884.90	3844.95	3831	3789.54
		A(GHZ)	8.09575	9.66979	9.57221	10.14535	9.897970	16.09782
		B(GHZ)	5.02094	4.34499	2.85116	4.48734	4.279850	2.00936
		C(GHZ)	3.94886	3.35233	2.36832	3.33119	3.337380	1.78638
		2D(GHZ)	4.452751	3.816522	2.598549	3.866288	3.77935	1.894592

Table S4: Rotational-Vibrational parameters of reactants, complexes and transition states obtained using M06-2X/6-311++G(3df,3pd) for OH•CHOH + O₂ + (FA) reaction

	c-Int-FA	c-Post-FA	t-TS-FA	t-Int-FA-1	trans-Post-FA-1	t-TS-FA-1	t-Int-FA-2	t-Post-FA-2	t-TS-FA-2	c-FA	t-FA	c-FA-FA	t-FA-FA
cm ⁻¹	46.07	28.78	894.33 <i>i</i>	26.92	27.1	941.09 <i>i</i>	34.19	36.81	866.9 <i>i</i>	514.2	650.15	42.09	50.86
cm ⁻¹	54.12	38.12	31.32	45.45	43.09	33.75	51.9	72.69	52.75	677.96	675.95	73.45	116.28
cm ⁻¹	119.71	52.21	40.92	71.3	49.47	60.07	121.28	74.32	58.43	1051.57	1071.55	103.82	131.78
cm ⁻¹	141.16	62.1	56.78	117.51	64.43	104.73	138.68	97.66	125.33	1143.42	1165.51	126.8	180.27
cm ⁻¹	158.47	66.87	63.93	134.17	113.73	121.24	175.87	129.13	163.24	1292.78	1323.24	161.07	200.65
cm ⁻¹	176.35	121.13	134.55	160.48	132.28	138.17	195.71	156.57	185.62	1429.08	1408.93	203.61	225.89
cm ⁻¹	190.28	124.92	139.92	168.5	152.76	154.59	228.89	175.78	221.38	1926.63	1874.24	369.51	344.54
cm ⁻¹	339.05	162.65	164.68	322.43	157.59	161.42	356.01	199.9	243.67	3041.9	3119.64	473.86	557.96
cm ⁻¹	346.45	211.46	329.32	381.12	170.61	329.73	473.44	236.6	328.98	3891.47	3809.13	558.71	702.85
cm ⁻¹	485.21	278.04	427.73	416.41	181.99	504.66	504.47	256.29	626.1			701.91	740.57
cm ⁻¹	517.46	296.58	625.1	505.85	252.16	594.79	610.08	291.73	637.85			819.07	899.54
cm ⁻¹	590.53	503.68	660.55	604.37	460.59	659.36	657.08	639.51	707.15			948.63	945.57
cm ⁻¹	692.77	564.59	694.68	650.94	677.46	681.05	705.91	708.68	717.29			1067.18	1066.04
cm ⁻¹	756.3	686.99	731.12	687.08	693.26	726.75	776.25	746.19	784.23			1070.75	1089.53
cm ⁻¹	817.67	695.63	748.81	811.73	740.31	767.96	882.24	966.85	905.14			1168.98	1182.93
cm ⁻¹	829.55	766.92	776.42	912.83	789.46	794.64	903.4	1036.33	958.75			1178.24	1262.99
cm ⁻¹	1059.02	1068.59	1070.21	1082.47	1085.95	1078.54	1067.15	1095.08	1099.26			1231.93	1267.46
cm ⁻¹	1094.76	1076.55	1102.29	1085.09	1106.32	1085.64	1089.23	1129.51	1145.16			1332.84	1405.74
cm ⁻¹	1155.14	1189.38	1160.92	1205.04	1180.11	1127.32	1233.91	1291.54	1204.25			1400.39	1423.85
cm ⁻¹	1198.75	1190.55	1184.7	1225.17	1223.49	1175.99	1270.9	1300.47	1257.9			1433.46	1437.7
cm ⁻¹	1263.66	1311.38	1188.79	1249.78	1282.71	1218.11	1287.55	1320.65	1271.76			1439.71	1451.48
cm ⁻¹	1283.1	1318.91	1285.41	1307.96	1335.24	1303.61	1307.18	1426.72	1364.58			1918.88	1822.7
cm ⁻¹	1340.2	1371.54	1366.3	1371.11	1382.17	1366.4	1361.02	1439.76	1386.06			3054.75	3126.02
cm ⁻¹	1403.25	1435.49	1383.66	1380.19	1423.29	1379.45	1409.24	1456.29	1412.76			3160.05	3148.89
cm ⁻¹	1424.11	1440.64	1399.7	1403.64	1435	1395.36	1445	1494.74	1439.39			3663.98	3420.76
cm ⁻¹	1443.61	1529.66	1435.55	1431.95	1458.29	1426.85	1480.99	1561.84	1467.15			3792.3	3550.88
cm ⁻¹	1474.93	1827.14	1642.29	1482.36	1848.56	1645.03	1488.16	1715.96	1587.3			3904.93	3909.13
cm ⁻¹	1912.5	1907.82	1905.18	1853.69	1853.68	1854.92	1823.26	1816.73	1808.38				
cm ⁻¹	3064.68	3034.54	1970.5	3132.49	3138.1	1945.63	3142.24	3057.57	1969.7				
cm ⁻¹	3164.18	3137.45	3033.99	3198.1	3194.12	3132.79	3157.84	3149.5	3150.54				
cm ⁻¹	3667.62	3529.56	3158.98	3637.2	3576.19	3241.43	3431.97	3188.19	3183.38				
cm ⁻¹	3719.8	3730.31	3726.42	3828.38	3678.21	3666.6	3509.07	3285.09	3259.77				
cm ⁻¹	3887.96	3864.44	3884.9	3844.93	3700.45	3813.32	3800.34	3444.42	3365.42				
A(GHZ)	3.42363	3.03514	4.37469	3.73068	4.12382	3.18437	3.1495	3.47685	3.21141	88.1342 1	78.2196 6	8.53655	5.71111
B(GHZ)	1.11163	0.6771	0.70108	0.87567	0.60269	1.14384	1.13587	0.78748	1.13033	11.8321 1	12.2394 8	1.35316	2.12645
C(GHZ)	1.02433	0.59081	0.63963	0.82827	0.52855	1.02662	1.04508	0.64206	1.01929	10.4316 5	10.5834 3	1.20838	1.59654
2D(GH Z)	1.0670876 1	0.63248 5	0.66965 1	0.8516402 94	0.56440 4	1.08364 6	1.0895297 2	0.7110621 69	1.07337 5	11.1098 3	11.3813 7	1.27872 3	1.84254 2

Table S5: T1 Diagnostic of each species involved in the reaction.

c-Int	c-TS	c-Post	t-Int	t-TS	t-Post
0.02323	0.02058	0.02375	0.02350	0.020738	0.02370

c-Int-FA	c-TS-FA	c-Post-FA	t-Int-FA	t-TS-FA	t-Post-FA
0.021689	0.01857	0.021643	0.021436(1)	0.019425(1)	0.02101(1)
			0.021660(2)	0.018970(2)	0.021783(2)

Table S6: Comparison between Calculated and Experimentally observed vibrational frequencies for formic acid and HO₂ radical.

Description	FA-Calculated	Experiment	Anharmonic-contribution		Scaled by 0.95
torsion	650.15	638	12.15	0.98	617.64
OCO bend	675.95	625	50.95	0.92	642.15
CH bend	1071.55	1033	38.55	0.96	1017.97
CO stretch	1165.51	1105	60.51	0.95	1107.23
OH bend	1323.24	1229	94.24	0.93	1257.08
CH bend	1408.93	1387	21.93	0.98	1338.48
C=O str	1874.24	1770	104.24	0.94	1780.53
CH stretch	3119.64	2943	176.64	0.94	2963.66
OH str	3809.13	3570	239.13	0.94	3618.67
			Average	0.9506936	
Description	HO ₂ -Calculated	Experiment	Anharmonic-contribution		
OH-Stretch	1273.03	1100.3	172.73	0.8643158	
OH-Bend	1471.36	1397.8	73.56	0.9500054	
O-O Stretch	3708.88	3415.1	293.78	0.9207901	
			Average	0.9117038	

Table S7: Calculated equilibrium constants (K_{eq} in $\text{cm}^3 \text{ molecule}^{-1}$) for the formation of two-body intermediate and complexes.

Temp	c-Int-unscaled	c-Int-scaled	t-Int-unscaled	t-Int-scaled	c-FA-FA	t-FA-FA
200	1.80E+18	<i>1.88E+18</i>	1.29E+14	<i>1.35E+14</i>	1.39E-21	6.09E-11
210	1.19E+16	<i>1.25E+16</i>	1.35E+12	<i>1.41E+12</i>	7.75E-22	9.82E-12
220	1.25E+14	<i>1.31E+14</i>	2.13E+10	<i>2.24E+10</i>	4.58E-22	1.88E-12
230	1.94E+12	<i>2.04E+12</i>	4.82E+08	<i>5.09E+08</i>	2.85E-22	4.15E-13
240	4.25E+10	<i>4.49E+10</i>	1.50E+07	<i>1.59E+07</i>	1.85E-22	1.05E-13
250	1.27E+09	<i>1.34E+09</i>	6.14E+05	<i>6.51E+05</i>	1.25E-22	2.95E-14
260	4.94E+07	<i>5.24E+07</i>	3.22E+04	<i>3.42E+04</i>	8.70E-23	9.19E-15
270	2.45E+06	<i>2.61E+06</i>	2.10E+03	<i>2.24E+03</i>	6.25E-23	3.13E-15
280	1.51E+05	<i>1.61E+05</i>	1.66E+02	<i>1.78E+02</i>	4.61E-23	1.16E-15
290	1.12E+04	<i>1.20E+04</i>	1.57E+01	<i>1.68E+01</i>	3.48E-23	4.57E-16
300	9.95E+02	<i>1.07E+03</i>	1.74E+00	<i>1.87E+00</i>	2.68E-23	1.93E-16
310	1.03E+02	<i>1.11E+02</i>	2.21E-01	<i>2.38E-01</i>	2.11E-23	8.64E-17
320	1.23E+01	<i>1.33E+01</i>	3.21E-02	<i>3.47E-02</i>	1.69E-23	4.07E-17

Table S8: Calculated equilibrium constants (K_{eq} in $\text{cm}^3 \text{ molecule}^{-1}$) for the formation of three-body complex.

Temp	c-Int ₀ -FA	t-Int ₁ -FA	t-Int ₂ -FA
200	1.10E+14	2.58E+11	8.26E+15
210	1.07E+12	4.01E+09	7.04E+13
220	1.60E+10	9.13E+07	9.25E+11
230	3.43E+08	2.89E+06	1.77E+10
240	1.01E+07	1.22E+05	4.71E+08
250	3.97E+05	6.64E+03	1.67E+07
260	2.00E+04	4.52E+02	7.68E+05
270	1.25E+03	3.77E+01	4.43E+04
280	9.56E+01	3.75E+00	3.13E+03
290	8.73E+00	4.38E-01	2.66E+02
300	9.36E-01	5.91E-02	2.66E+01
310	1.16E-01	9.09E-03	3.09E+00
320	1.64E-02	1.57E-03	4.11E-01

Table S9: Calculated standard entropy of each species (in $\text{calK}^{-1}\text{mol}^{-1}$).

c-Int	c-TS	c-Post	t-Int	t-TS	t-Post
73.665	72.016	82.718	73.548	71.958	82.675

c-Int-FA	c-TS-FA	c-Post-FA	t-Int-FA	t-TS-FA	t-Post-FA
98.748	103.621	112.365	102.82 (1)	99.239 (1)	111.949 (1)
			97.715 (2)	94.788 (2)	104.828 (2)

Table S10: Comparison of rate constant (s^{-1}) using CVT/SCT (from Polyrate and GaussRate Program and RRKM/Eckart (from MultiWell) calculations.

	CVT/SCT			RRKM/Eckart		
Temp	cis	Trans-1	Trans-2	cis	Trans-1	Trans-2
200	3.16E+04	1.40E+04	1.68E+07	3.79E+04	1.05E+05	4.20E+07
210	8.60E+04	3.47E+04	3.02E+07	8.83E+04	1.94E+05	6.45E+07
220	2.16E+05	7.92E+04	5.15E+07	1.95E+05	3.48E+05	9.61E+07
230	5.02E+05	1.68E+05	8.39E+07	4.10E+05	6.05E+05	1.39E+08
240	1.10E+06	3.36E+05	1.31E+08	8.20E+05	1.02E+06	1.97E+08
250	2.26E+06	6.35E+05	1.98E+08	1.57E+06	1.67E+06	2.72E+08
260	4.41E+06	1.14E+06	2.90E+08	2.89E+06	2.65E+06	3.67E+08
270	8.23E+06	1.97E+06	4.13E+08	5.10E+06	4.10E+06	4.87E+08
280	1.47E+07	3.26E+06	5.73E+08	8.71E+06	6.18E+06	6.35E+08
290	2.54E+07	5.22E+06	7.77E+08	1.44E+07	9.11E+06	8.15E+08
300	4.22E+07	8.10E+06	1.03E+09	2.31E+07	1.31E+07	1.03E+09
310	6.81E+07	1.22E+07	1.35E+09	3.61E+07	1.86E+07	1.28E+09
320	1.07E+08	1.80E+07	1.73E+09	5.50E+07	2.57E+07	1.58E+09

Table S11 (a): Unimolecular rate constant (s^{-1}) for $\text{cis-Int}_0\text{FA} \rightarrow \text{cis-Post}_0\text{FA}$ calculated using Polyrate and GaussRate Program.

T(K)	TST	CVT	CVT/ZCT	CVT/SCT	Variaional effect ($k_{\text{CVT}}/k_{\text{TST}}$)	SCT-Tunneling Γ
200	1.13E+04	1.12E+04	1.74E+04	3.16E+04	0.99	2.82
210	3.44E+04	3.41E+04	5.05E+04	8.60E+04	0.99	2.52
220	9.46E+04	9.39E+04	1.34E+05	2.16E+05	0.99	2.30
230	2.39E+05	2.37E+05	3.26E+05	5.02E+05	0.99	2.12
240	5.59E+05	5.54E+05	7.40E+05	1.10E+06	0.99	1.99
250	1.22E+06	1.21E+06	1.58E+06	2.26E+06	0.99	1.87
260	2.52E+06	2.50E+06	3.18E+06	4.41E+06	0.99	1.76
270	4.92E+06	4.88E+06	6.09E+06	8.23E+06	0.99	1.69
280	9.18E+06	9.08E+06	1.12E+07	1.47E+07	0.99	1.62
290	1.64E+07	1.62E+07	1.96E+07	2.54E+07	0.99	1.57
300	2.82E+07	2.79E+07	3.33E+07	4.22E+07	0.99	1.51
310	4.68E+07	4.63E+07	5.46E+07	6.81E+07	0.99	1.47
320	7.54E+07	7.45E+07	8.68E+07	1.07E+08	0.99	1.44

Table S11 (b): Unimolecular rate constant (s^{-1}) for $\text{trans-Int}_1\text{fA} \rightarrow \text{trans-Post}_1\text{-fA}$ calculated using Polyrate and GaussRate Program.

T(K)	TST	CVT	CVT/ZCT	CVT/SCT	$k_{\text{CVT}}/k_{\text{TST}}$	Γ
200	1.40E+04	2.34E+04	4.27E+04	1.13E+05	1.67	4.83
210	3.47E+04	5.81E+04	9.96E+04	2.36E+05	1.67	4.06
220	7.92E+04	1.33E+05	2.16E+05	4.69E+05	1.68	3.53
230	1.68E+05	2.83E+05	4.39E+05	8.84E+05	1.68	3.12
240	3.36E+05	5.66E+05	8.44E+05	1.59E+06	1.68	2.81
250	6.35E+05	1.07E+06	1.54E+06	2.75E+06	1.69	2.57
260	1.14E+06	1.93E+06	2.70E+06	4.58E+06	1.69	2.37
270	1.97E+06	3.33E+06	4.53E+06	7.38E+06	1.69	2.22
280	3.26E+06	5.52E+06	7.35E+06	1.15E+07	1.69	2.08
290	5.22E+06	8.84E+06	1.15E+07	1.75E+07	1.69	1.98
300	8.10E+06	1.37E+07	1.76E+07	2.59E+07	1.69	1.89
310	1.22E+07	2.07E+07	2.61E+07	3.74E+07	1.70	1.81
320	1.80E+07	3.05E+07	3.78E+07	5.29E+07	1.69	1.73

Table S11 (c): Unimolecular rate constant (s^{-1}) for $\text{trans-Int}_2\text{fA} \rightarrow \text{trans-Post2-FA}$ calculated using Polyrate and GaussRate Program.

T(K)	TST	CVT	CVT/ZCT	CVT/SCT	kCVT/kTST	Γ
200	1.68E+07	1.58E+07	3.14E+07	6.05E+07	0.94	3.83
210	3.02E+07	2.85E+07	5.30E+07	9.58E+07	0.94	3.36
220	5.15E+07	4.87E+07	8.56E+07	1.46E+08	0.95	3.00
230	8.39E+07	7.94E+07	1.33E+08	2.17E+08	0.95	2.73
240	1.31E+08	1.24E+08	2.00E+08	3.13E+08	0.95	2.52
250	1.98E+08	1.88E+08	2.91E+08	4.39E+08	0.95	2.34
260	2.90E+08	2.76E+08	4.12E+08	6.03E+08	0.95	2.18
270	4.13E+08	3.93E+08	5.70E+08	8.11E+08	0.95	2.06
280	5.73E+08	5.46E+08	7.72E+08	1.07E+09	0.95	1.96
290	7.77E+08	7.41E+08	1.02E+09	1.39E+09	0.95	1.88
300	1.03E+09	9.86E+08	1.33E+09	1.77E+09	0.96	1.80
310	1.35E+09	1.29E+09	1.71E+09	2.23E+09	0.96	1.73
320	1.73E+09	1.65E+09	2.15E+09	2.76E+09	0.95	1.67

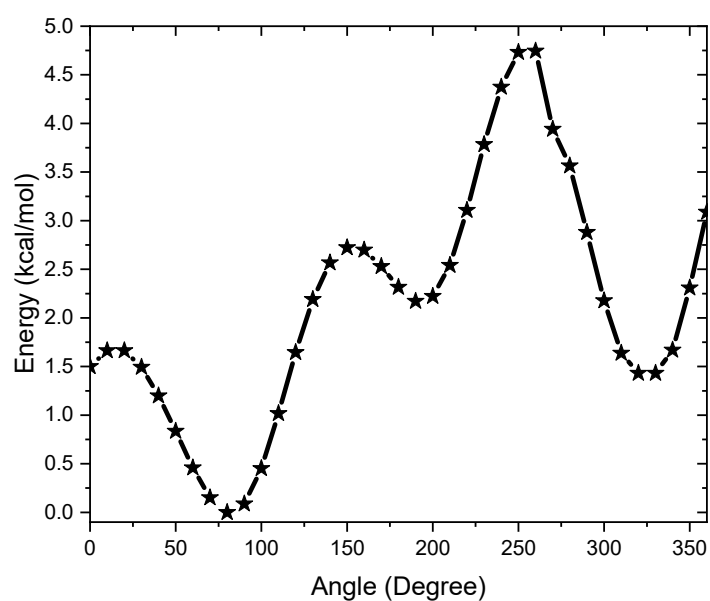


Figure S1 (a) Hindered Rotor potential for cis-OHCH(OO)OH.

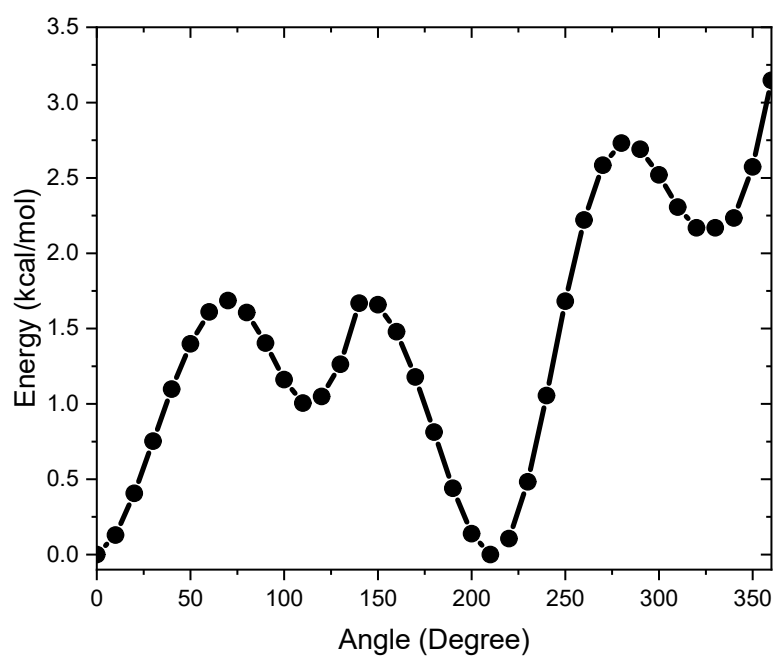


Figure S1 (b) Hindered Rotor potential for trans-OHCH(OO)OH

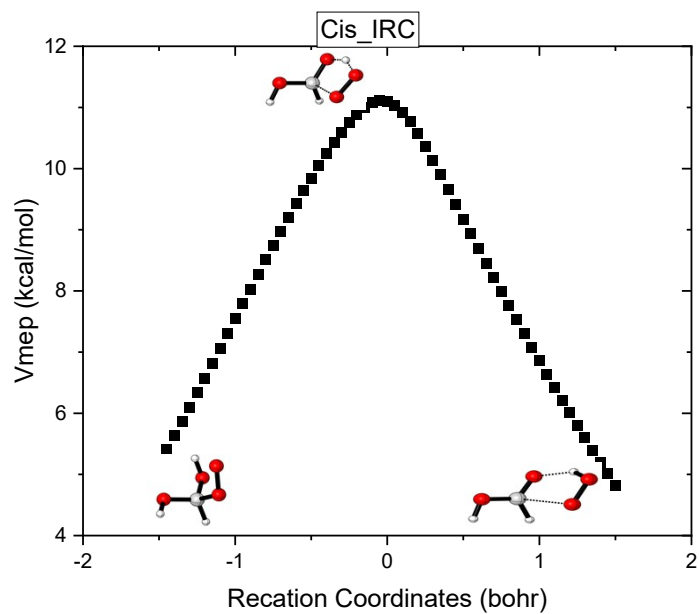


Figure S2(a). IRC calculation for cis Intermediate going to Post-Intermediate without FA computed at M06-2X/6-311++G(3df,3pd).

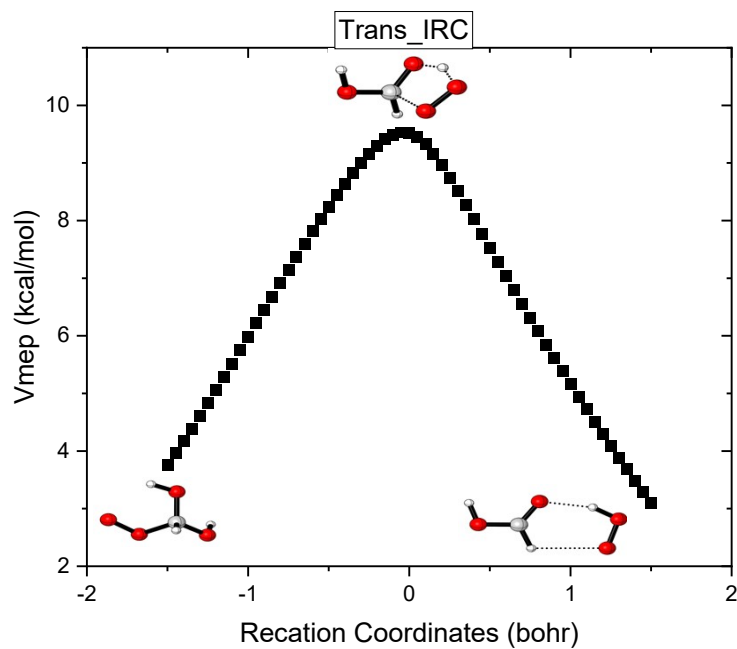


Figure S2(b). IRC calculation for trans Intermediate going to trans-Post-Intermediate without FA computed at M06-2X/6-311++G(3df,3pd).

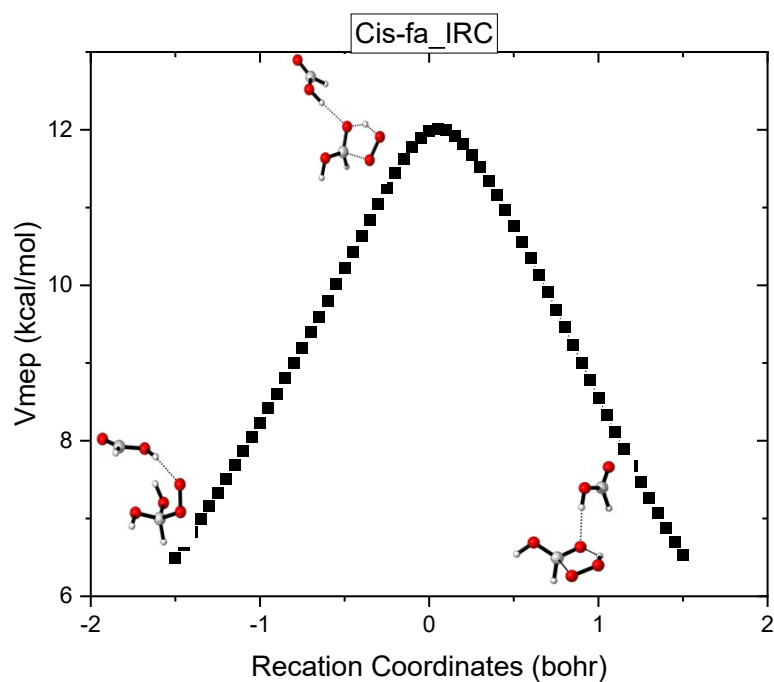


Figure S3(a). IRC calculation for cis Intermediate going to cis-Post-Intermediate with the effect of FA computed at M06-2X/6-311++G(3df,3pd).

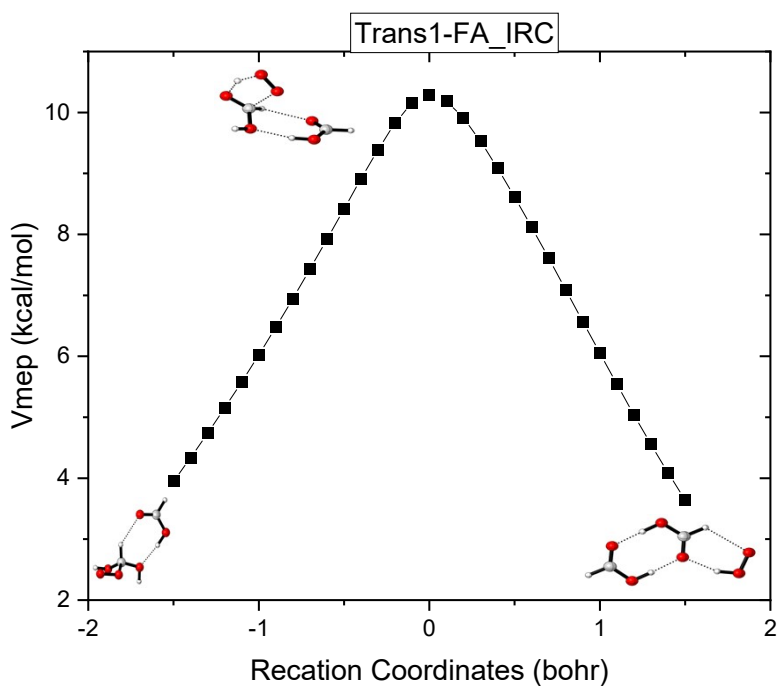


Figure S3(b). IRC calculation for trans-1 Intermediate going to trans-1Post-Intermediate with the effect of FA computed at M06-2X/6-311++G(3df,3pd).

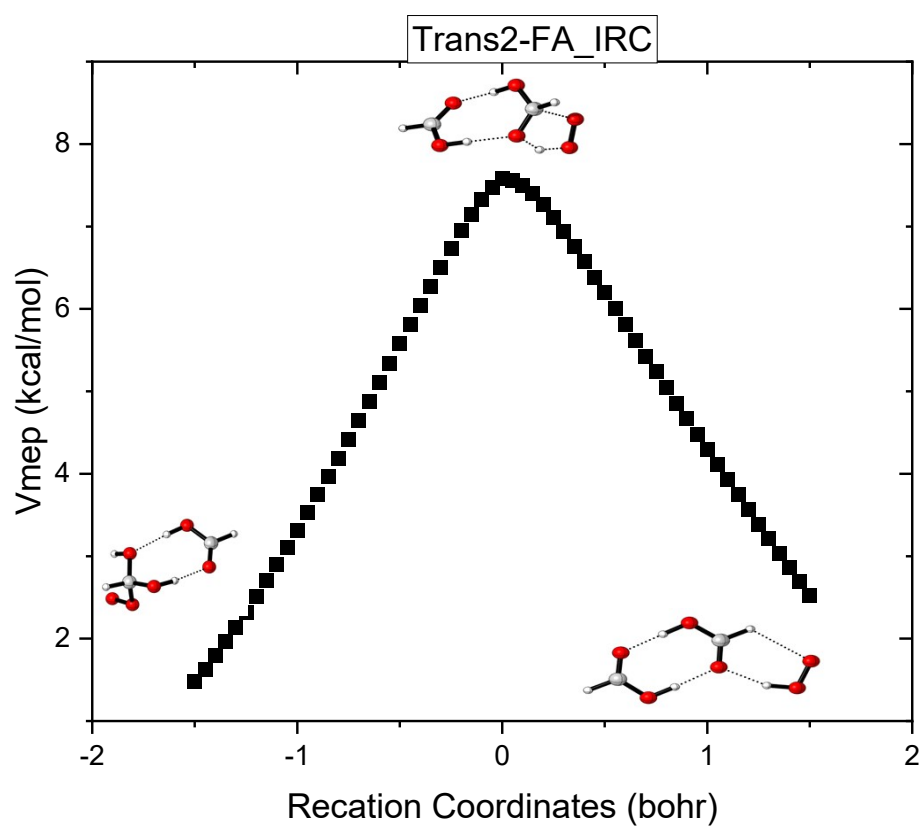


Figure S3(c). IRC calculation for trans-2 Intermediate going to trans-2-Post-Intermediate with the effect of FA computed at M06-2X/6-311++G(3df,3pd).

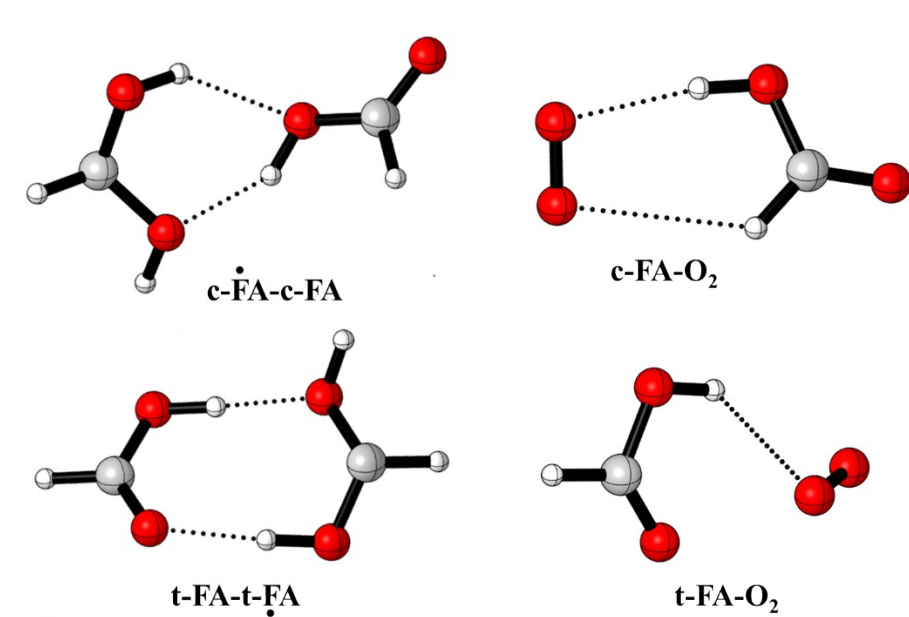


Figure S4. The possible number of pathways for the collision of two molecules leading to the formation of two-body complex.

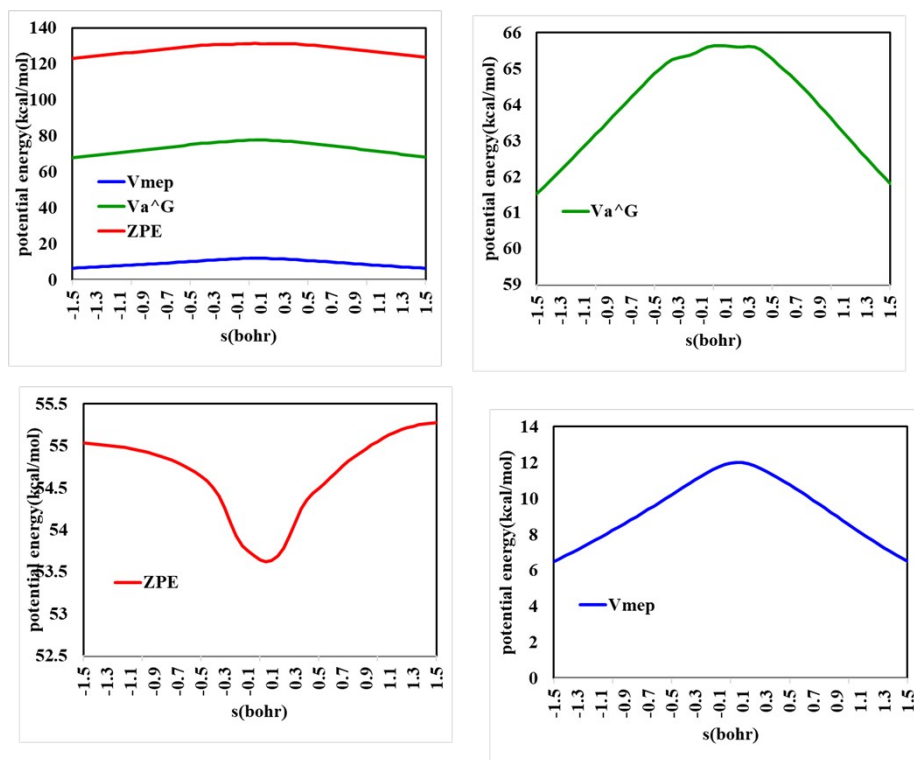


Figure S5 (a) V_{mep} , ZPE and V_a^G as a function of s for $\text{cis-Int0-FA} \rightarrow \text{cis-Post0-FA}$ calculated at M06-2X/6-311++G(3df,3pd)

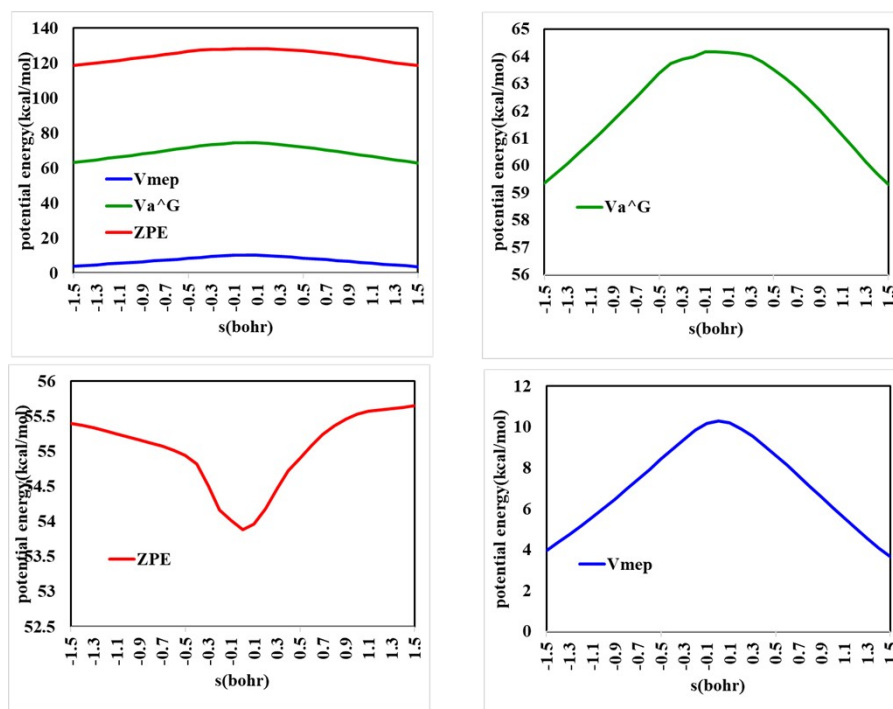


Figure S5 (b) V_{mep} , ZPE and V_a^G as a function of s for $\text{trans-Int1-FA} \rightarrow \text{trans-Post1-FA}$ calculated at M06-2X/6-311++G(3df,3pd).

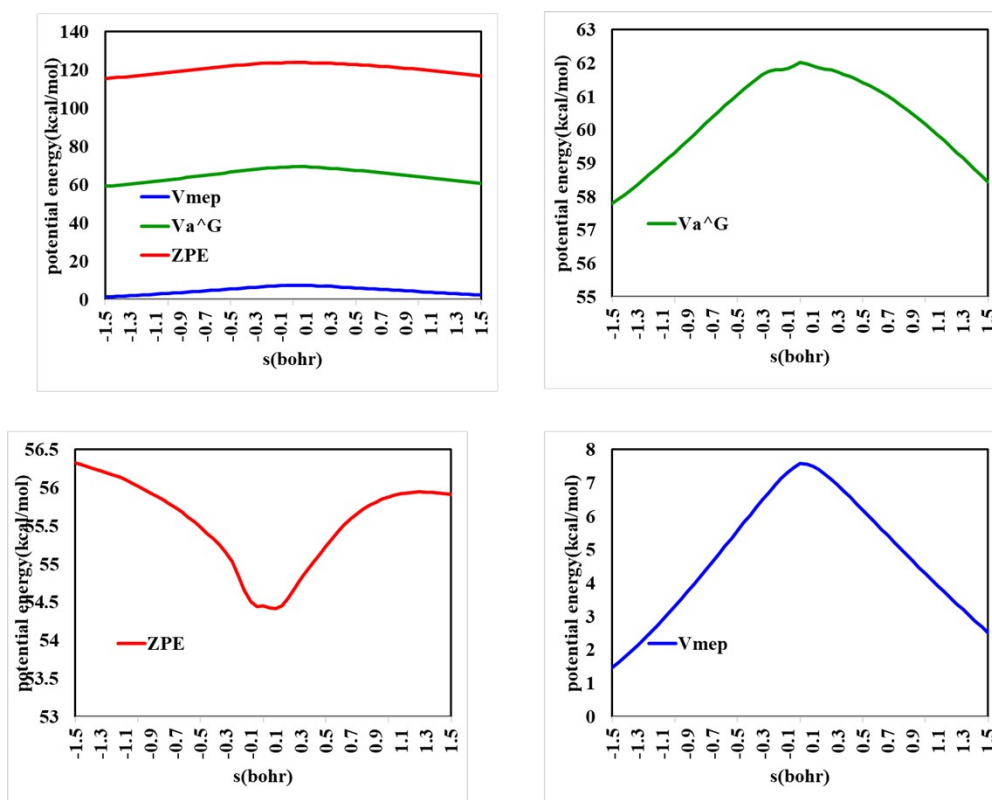


Figure S5 (c) V_{mep} , ZPE and V_a^G as a function of s for trans-Int2-FA $\rightarrow$ trans-Post₂-FA calculated at M06-2X/6-311++G(3df,3pd).

MultiWell Input files for O₂ + •CHOHOH at 300 K.

O₂ + •CHOHOH system (cis)

10. 500 5000 85000. 2113989025

'BAR' 'KCAL' 'GHZ'

300 300

6

0.0001 0.001 0.01 0.1 1. 10. !Pressure

2 2

1 'c-Int' -41.2 4.452750737 1 1 2 !OOCH₃

2 'c-Post' -42.6 2.598549451 1 1 2 !HOCH₂O

3 'c-FA+O₂' 0.0

4 'c-fa_HO₂' -39.4

3.75 82. 28. 79. ! N₂ collider

1 5.4 400. 1 300.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 ! L-J surrogate: n-butane
'LJ'

2 5.4 400. 1 300.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 ! L-J surrogate: n-butane
'LJ'

3

1 3 'TS0' 1.0 1 1 1 1.0e+16 41.2 'REV' 'FAST' 'NOTUN' 'NOCENT' 'ILT'

1 2 'c-TS' 3.81652202 1 1 1 1.1e+13 6.7 'REV' 'FAST' 'TUN' 'NOCENT' 'SUM'
'TUN' 915

2 4 'TS0-p' 1.0 1 1 1 1.0e+16 4.0 'REV' 'FAST' 'NOTUN' 'NOCENT' 'ILT'

100000 'COLL' 100. 'CHEMACT' 1 3 0.

O2 + •CHOHOH system (trans)

10. 500 5000 85000. 2113989025

'BAR' 'KCAL' 'GHZ'

300 300

6

0.0001 0.001 0.01 0.1 1. 10.

2 2

1 't-Int' -37.4 3.866287901 1 1 2 ! OCH3

2 't-Post' -45.2 1.894592441 1 1 2 ! HOCH2O

3 't-FA+O2' 0.0

4 't-fa_HO2' -33.1

3.75 82. 28. 79. ! N2 collider

1 5.4 400. 1 310.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 ! L-J surrogate: n-butane
'LJ'

2 5.4 400. 1 310.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 ! L-J surrogate: n-butane
'LJ'

3

1 3 'TS0' 1.0 1 1 1 1.0e+16 37.4 'REV' 'FAST' 'NOTUN' 'NOCENT' 'ILT'
1 2 't-TS' 3.779349917 1 1 1 1.1e+13 8.2 'REV' 'FAST' 'TUN' 'NOCENT'
'SUM'

'TUN' 948

2 4 'TS0-p' 1.0 1 1 1 1.0e+16 12 'REV' 'FAST' 'NOTUN' 'NOCENT' 'ILT'

100000 'COLL' 100. 'CHEMACT' 1 3 0.

MultiWell Input files for O₂ + •CHOHOH (+ FA)

O2 + •CHOHOH system (cis)

10. 500 5000 85000. 2113989025

'BAR' 'KCAL' 'GHZ'

300 300

6
0.0001 0.001 0.01 0.1 1. 10.

2 2
1 'c-Int-FA' -37.9 1.067087606 1 1 2 ! OCH₃
2 'c-Post-FA' -39.4 0.632485139 1 1 2 ! HOCH₂O
3 'c-FAFA+O₂' 0.0
4 'c-fa_HO₂' -33.1

3.75 82. 28. 79. ! N₂ collider
1 5.4 400. 1 310.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 ! L-J surrogate: n-butane
'LJ'
2 5.4 400. 1 310.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 ! L-J surrogate: n-butane
'LJ'

3
1 3 'TS0' 1.0 1 1 1 1.0e+16 37.9 'REV' 'FAST' 'NOTUN' 'NOCENT' 'ILT' !
nominal Ea = 41.2
1 2 'c-TS-FA' 0.669650506 1 1 1 1.1e+13 8.7 'REV' 'FAST' 'TUN' 'NOCENT'
'SUM'
'TUN' 894
2 4 'TS0-p' 1.0 1 1 1 1.0e+16 8 'REV' 'FAST' 'NOTUN' 'NOCENT' 'ILT'

100000 'COLL' 100. 'CHEMACT' 1 3 0.

O₂ + •CHOHOH system (trans-1)

10. 500 5000 85000. 2113989025
'BAR' 'KCAL' 'GHZ'
300 300

6
0.0001 0.001 0.01 0.1 1. 10.

2 2
1 't-Int-FA1' -34.5 0.851640294 1 1 2 ! OCH₃
2 't-Int-Pol' -48.5 0.564403933 1 1 2 ! OCH₃
3 't-FA+O₂' 0.0
4 't-fa_HO₂' -39.4

3.75 82. 28. 79. ! N₂ collider
1 5.4 400. 1 30.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 ! L-J surrogate: n-butane
'LJ'
2 5.4 400. 1 200.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 ! L-J surrogate: n-butane
'LJ'

3

1 3 'TS01' 1.0 1 1 1 1.0e+16 34.5 'REV' 'FAST' 'NOTUN' 'NOCENT' 'ILT'
 1 2 't-TS1FA' 1.08364617 1 1 1 1.1e+13 7.4 'REV' 'FAST' 'TUN' 'NOCENT'
 'SUM'
 'TUN' 941
 2 4 'TS0-p1' 1.0 1 1 1 1.0e+16 9.1 'REV' 'FAST' 'NOTUN' 'NOCENT' 'ILT'
 100000 'COLL' 100. 'CHEMACT' 1 3 0.

O2 + •CHOHOH system (trans-2)

10. 500 5000 85000. 2113989025

'BAR' 'KCAL' 'GHZ'

375 375

6

0.0001 0.001 0.01 0.1 1. 10.

2 2

1 't-Int-FA2' -39.2 1.089529724 1 1 2 !HOCH2O

2 't-Int-Po2' -38.1 0.711062169 1 1 2 !HOCH2O

3 't-FA+O2' 0.0

4 't-fa_HO2' -39.4

3.75 82. 28. 79. !N2 collider

1 5.4 400. 1 300.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 !L-J surrogate: n-butane
 'LJ'

2 5.4 400. 1 300.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 !L-J surrogate: n-butane
 'LJ'

3

1 3 'TS02' 1.0 1 1 1 1.0e+16 39.2 'REV' 'FAST' 'NOTUN' 'NOCENT' 'ILT'
 !

1 2 't-TS2FA' 1.073375082 1 1 1 1.1e+13 4.7 'REV' 'FAST' 'TUN' 'NOCENT'
 'SUM'

'TUN' 867

2 4 'TS0-p2' 1.0 1 1 1 1.0e+16 1.3 'REV' 'FAST' 'NOTUN' 'NOCENT' 'ILT'

100000 'COLL' 100. 'CHEMACT' 1 3 0.

Cis-FA+cis-CHOHOH → cis-CHOHOH-FA (Ke)

KCAL MCC

13 ! Nt number of temperatures

200. 210. 220. 230. 240. 250. 260. 270. 280. 290. 300. 310. 320

3

reac cis-CHOHOH_____ 0.0

CHOHOH

! NIST / JANAF 1998

! enthalpy from Ruscic et al., J. Phys. Chem. A, 2006, 110 (21), 6592-6601

! (blank comment line)

1 1 1

0.0 2

14 'HAR' 'GHZ'

| | | | | |
|----|-----|-------------|---|---|
| 1 | vib | 248.57 0 | 1 | |
| 2 | vib | 381 0 | 1 | |
| 3 | vib | 547.4 0 | 1 | |
| 4 | vib | 951.93 0 | 1 | |
| 5 | vib | 1097.35 | 0 | 1 |
| 6 | vib | 1133.16 | 0 | 1 |
| 7 | vib | 1248.19 | 0 | 1 |
| 8 | vib | 1357.65 | 0 | 1 |
| 9 | vib | 1439.75 | 0 | 1 |
| 10 | vib | 3050.1 0 | 1 | |
| 11 | vib | 3930.03 | 0 | 1 |
| 12 | vib | 3930.4 0 | 1 | |
| 13 | qro | 62.41178 | 1 | 1 |
| 14 | qro | 10.09968641 | 1 | 2 |

reac HCOOH_____ 0.0

HCOOH

! NIST / JANAF 1998

! (blank comment line)

! (blank comment line)

1 1 1

0.0 1

11 'HAR' 'GHZ'

| | | | | |
|---|-----|----------|---|---|
| 1 | vib | 514.2 0 | 1 | |
| 2 | vib | 677.96 0 | 1 | |
| 3 | vib | 1051.57 | 0 | 1 |
| 4 | vib | 1143.42 | 0 | 1 |
| 5 | vib | 1292.78 | 0 | 1 |
| 6 | vib | 1429.08 | 0 | 1 |

| | | | | |
|----|-----|-------------|---|---|
| 7 | vib | 1926.63 | 0 | 1 |
| 8 | vib | 3041.9 0 | 1 | |
| 9 | vib | 3891.47 | 0 | 1 |
| 10 | qro | 88.13421 | 1 | 1 |
| 11 | qro | 11.10983484 | 1 | 2 |

prod cis-CHOHOH-FA_____ -5.1

CHOHOHHCOOH

! NIST / JANAF 1998

! enthalpy from Ruscic et al., J. Phys. Chem. A, 2006, 110 (21), 6592-6601

! (blank comment line)

1 1 1

0.0 2

29 'HAR' 'GHZ'

| | | | | |
|----|-----|-------------|---|---|
| 1 | vib | 42.09 0 | 1 | |
| 2 | vib | 73.45 0 | 1 | |
| 3 | vib | 103.82 0 | 1 | |
| 4 | vib | 126.8 0 | 1 | |
| 5 | vib | 161.07 0 | 1 | |
| 6 | vib | 203.61 0 | 1 | |
| 7 | vib | 369.51 0 | 1 | |
| 8 | vib | 473.86 0 | 1 | |
| 9 | vib | 558.71 0 | 1 | |
| 10 | vib | 701.91 0 | 1 | |
| 11 | vib | 819.07 0 | 1 | |
| 12 | vib | 948.63 0 | 1 | |
| 13 | vib | 1067.18 | 0 | 1 |
| 14 | vib | 1070.75 | 0 | 1 |
| 15 | vib | 1168.98 | 0 | 1 |
| 16 | vib | 1178.24 | 0 | 1 |
| 17 | vib | 1231.93 | 0 | 1 |
| 18 | vib | 1332.84 | 0 | 1 |
| 19 | vib | 1400.39 | 0 | 1 |
| 20 | vib | 1433.46 | 0 | 1 |
| 21 | vib | 1439.71 | 0 | 1 |
| 22 | vib | 1918.88 | 0 | 1 |
| 23 | vib | 3054.75 | 0 | 1 |
| 24 | vib | 3160.05 | 0 | 1 |
| 25 | vib | 3663.98 | 0 | 1 |
| 26 | vib | 3792.3 0 | 1 | |
| 27 | vib | 3904.93 | 0 | 1 |
| 28 | qro | 8.53655 | 1 | 1 |
| 29 | qro | 1.278722597 | 1 | 2 |

cis-CHOH₂OH-FA+O₂→ cis-CHOH(OO)OH-FA (Ke)

KCAL MCC

13 ! Nt number of temperatures

200. 210. 220. 230. 240. 250. 260. 270. 280. 290. 300. 310. 320

3

reac cis-CHOH₂OH-FA_____ 0.0

CHOH₂OHCOOH

! NIST / JANAF 1998

! enthalpy from Ruscic et al., J. Phys. Chem. A, 2006, 110 (21), 6592-6601

! (blank comment line)

1 1 1

0.0 2

29 'HAR' 'GHZ'

| | | | | |
|----|-----|-------------|---|---|
| 1 | vib | 42.09 | 0 | 1 |
| 2 | vib | 73.45 | 0 | 1 |
| 3 | vib | 103.82 | 0 | 1 |
| 4 | vib | 126.8 | 0 | 1 |
| 5 | vib | 161.07 | 0 | 1 |
| 6 | vib | 203.61 | 0 | 1 |
| 7 | vib | 369.51 | 0 | 1 |
| 8 | vib | 473.86 | 0 | 1 |
| 9 | vib | 558.71 | 0 | 1 |
| 10 | vib | 701.91 | 0 | 1 |
| 11 | vib | 819.07 | 0 | 1 |
| 12 | vib | 948.63 | 0 | 1 |
| 13 | vib | 1067.18 | 0 | 1 |
| 14 | vib | 1070.75 | 0 | 1 |
| 15 | vib | 1168.98 | 0 | 1 |
| 16 | vib | 1178.24 | 0 | 1 |
| 17 | vib | 1231.93 | 0 | 1 |
| 18 | vib | 1332.84 | 0 | 1 |
| 19 | vib | 1400.39 | 0 | 1 |
| 20 | vib | 1433.46 | 0 | 1 |
| 21 | vib | 1439.71 | 0 | 1 |
| 22 | vib | 1918.88 | 0 | 1 |
| 23 | vib | 3054.75 | 0 | 1 |
| 24 | vib | 3160.05 | 0 | 1 |
| 25 | vib | 3663.98 | 0 | 1 |
| 26 | vib | 3792.3 | 0 | 1 |
| 27 | vib | 3904.93 | 0 | 1 |
| 28 | qro | 8.53655 | 1 | 1 |
| 29 | qro | 1.278722597 | 1 | 2 |

```

reac  O2_____ 0.0
O2
! NIST / JANAF 1998
! (blank comment line)
! (blank comment line)
2  1  4
0.0  3
7882.39 2
13120.9 1
32664.1 1
2  'HAR' 'GHZ'
1  vib  1778.6  0 1
2  qro  44.798983 1 2

```

```

prod  cis-Int-FA_____ -37.96
HCOOHCHOHOHO2
! NIST / JANAF 1998
! enthalpy from Ruscic et al., J. Phys. Chem. A, 2006, 110 (21), 6592-6601
! (blank comment line)
1  1  1
0.0  2
35  'HAR' 'GHZ'
1  vib  46.07  0 1
2  vib  54.12  0 1
3  vib  119.71 0 1
4  vib  141.16 0 1
5  vib  158.47 0 1
6  vib  176.35 0 1
7  vib  190.28 0 1
8  vib  339.05 0 1
9  vib  346.45 0 1
10 vib  485.21 0 1
11 vib  517.46 0 1
12 vib  590.53 0 1
13 vib  692.77 0 1
14 vib  756.3  0 1
15 vib  817.67 0 1
16 vib  829.55 0 1
17 vib  1059.02 0 1
18 vib  1094.76 0 1
19 vib  1155.14 0 1
20 vib  1198.75 0 1
21 vib  1263.66 0 1
22 vib  1283.1 0 1
23 vib  1340.2 0 1
24 vib  1403.25 0 1

```

| | | | | |
|----|-----|-------------|---|---|
| 25 | vib | 1424.11 | 0 | 1 |
| 26 | vib | 1443.61 | 0 | 1 |
| 27 | vib | 1474.93 | 0 | 1 |
| 28 | vib | 1912.5 0 | 1 | |
| 29 | vib | 3064.68 | 0 | 1 |
| 30 | vib | 3164.18 | 0 | 1 |
| 31 | vib | 3667.62 | 0 | 1 |
| 32 | vib | 3719.8 0 | 1 | |
| 33 | vib | 3887.96 | 0 | 1 |
| 34 | qro | 3.42363 | 1 | 1 |
| 35 | qro | 1.067087606 | 1 | 2 |

trans-FA+trans-CHOHOH →trans-CHOHOH-FA (Ke)

KCAL MCC

13 ! Nt number of temperatures

200. 210. 220. 230. 240. 250. 260. 270. 280. 290. 300. 310. 320

3

reac trans-CHOHOH_____ 0.0

CHOHOH

! NIST / JANAF 1998

! enthalpy from Ruscic et al., J. Phys. Chem. A, 2006, 110 (21), 6592-6601

! (blank comment line)

1 1 1

0.0 2

14 'HAR' 'GHZ'

| | | | | |
|---|-----|----------|---|---|
| 1 | vib | 298.39 0 | 1 | |
| 2 | vib | 368.08 0 | 1 | |
| 3 | vib | 553.33 0 | 1 | |
| 4 | vib | 956.68 0 | 1 | |
| 5 | vib | 1092 0 | 1 | |
| 6 | vib | 1165.53 | 0 | 1 |
| 7 | vib | 1220.29 | 0 | 1 |

| | | | | |
|----|-----|-------------|---|---|
| 8 | vib | 1373.81 | 0 | 1 |
| 9 | vib | 1426.02 | 0 | 1 |
| 10 | vib | 3136.7 0 | 1 | |
| 11 | vib | 3880.88 | 0 | 1 |
| 12 | vib | 3923.65 | 0 | 1 |
| 13 | qro | 57.23206 | 1 | 1 |
| 14 | qro | 10.20036475 | 1 | 2 |

reac t-HCOOH_____ 0.0

HCOOH

! NIST / JANAF 1998

! (blank comment line)

! (blank comment line)

1 1 1

0.0 1

11 'HAR' 'GHZ'

| | | | | |
|----|-----|-------------|---|---|
| 1 | vib | 650.15 0 | 1 | |
| 2 | vib | 675.95 0 | 1 | |
| 3 | vib | 1071.55 | 0 | 1 |
| 4 | vib | 1165.51 | 0 | 1 |
| 5 | vib | 1323.24 | 0 | 1 |
| 6 | vib | 1408.93 | 0 | 1 |
| 7 | vib | 1874.24 | 0 | 1 |
| 8 | vib | 3119.64 | 0 | 1 |
| 9 | vib | 3809.13 | 0 | 1 |
| 10 | qro | 78.21966 | 1 | 1 |
| 11 | qro | 11.38137425 | 1 | 2 |

prod trans-CHOHOH-FA_____ -15.3

CHOHOHHCOOH

! NIST / JANAF 1998

! enthalpy from Ruscic et al., J. Phys. Chem. A, 2006, 110 (21), 6592-6601

! (blank comment line)

1 1 1

0.0 2

29 'HAR' 'GHZ'

| | | | | |
|----|-----|----------|---|---|
| 1 | vib | 50.86 0 | 1 | |
| 2 | vib | 116.28 0 | 1 | |
| 3 | vib | 131.78 0 | 1 | |
| 4 | vib | 180.27 0 | 1 | |
| 5 | vib | 200.65 0 | 1 | |
| 6 | vib | 225.89 0 | 1 | |
| 7 | vib | 344.54 0 | 1 | |
| 8 | vib | 557.96 0 | 1 | |
| 9 | vib | 702.85 0 | 1 | |
| 10 | vib | 740.57 0 | 1 | |
| 11 | vib | 899.54 0 | 1 | |
| 12 | vib | 945.57 0 | 1 | |
| 13 | vib | 1066.04 | 0 | 1 |
| 14 | vib | 1089.53 | 0 | 1 |
| 15 | vib | 1182.93 | 0 | 1 |
| 16 | vib | 1262.99 | 0 | 1 |
| 17 | vib | 1267.46 | 0 | 1 |
| 18 | vib | 1405.74 | 0 | 1 |
| 19 | vib | 1423.85 | 0 | 1 |
| 20 | vib | 1437.7 0 | 1 | |
| 21 | vib | 1451.48 | 0 | 1 |
| 22 | vib | 1822.7 0 | 1 | |

| | | | | |
|----|-----|-------------|---|---|
| 23 | vib | 3126.02 | 0 | 1 |
| 24 | vib | 3148.89 | 0 | 1 |
| 25 | vib | 3420.76 | 0 | 1 |
| 26 | vib | 3550.88 | 0 | 1 |
| 27 | vib | 3909.13 | 0 | 1 |
| 28 | qro | 5.71111 | 1 | 1 |
| 29 | qro | 1.842542397 | 1 | 2 |

trans-CHOHOH-FA+O2→ trans1-CHOH(OO)OH-FA(Ke)

KCAL MCC

13 ! Nt number of temperatures

200. 210. 220. 230. 240. 250. 260. 270. 280. 290. 300. 310. 320

3

reac trans-CHOHOH-FA_____ 0.0

CHOHOHHCOOH

! NIST / JANAF 1998

! enthalpy from Ruscic et al., J. Phys. Chem. A, 2006, 110 (21), 6592-6601

! (blank comment line)

1 1 1

0.0 2

29 'HAR' 'GHZ'

1 vib 50.86 0 1

2 vib 116.28 0 1

3 vib 131.78 0 1

4 vib 180.27 0 1

5 vib 200.65 0 1

| | | | | |
|----|-----|-------------|---|---|
| 6 | vib | 225.89 0 | 1 | |
| 7 | vib | 344.54 0 | 1 | |
| 8 | vib | 557.96 0 | 1 | |
| 9 | vib | 702.85 0 | 1 | |
| 10 | vib | 740.57 0 | 1 | |
| 11 | vib | 899.54 0 | 1 | |
| 12 | vib | 945.57 0 | 1 | |
| 13 | vib | 1066.04 | 0 | 1 |
| 14 | vib | 1089.53 | 0 | 1 |
| 15 | vib | 1182.93 | 0 | 1 |
| 16 | vib | 1262.99 | 0 | 1 |
| 17 | vib | 1267.46 | 0 | 1 |
| 18 | vib | 1405.74 | 0 | 1 |
| 19 | vib | 1423.85 | 0 | 1 |
| 20 | vib | 1437.7 0 | 1 | |
| 21 | vib | 1451.48 | 0 | 1 |
| 22 | vib | 1822.7 0 | 1 | |
| 23 | vib | 3126.02 | 0 | 1 |
| 24 | vib | 3148.89 | 0 | 1 |
| 25 | vib | 3420.76 | 0 | 1 |
| 26 | vib | 3550.88 | 0 | 1 |
| 27 | vib | 3909.13 | 0 | 1 |
| 28 | qro | 5.71111 | 1 | 1 |
| 29 | qro | 1.842542397 | 1 | 2 |

reac O2_____ 0.0

O2

! NIST / JANAF 1998

! (blank comment line)

! (blank comment line)

2 1 4

0.0 3

7882.39 2

13120.9 1

32664.1 1

2 'HAR' 'GHZ'

1 vib 1778.6 0 1

2 qro 44.798983 1 2

prod tInt1FA_____ -34.5

HCOOHCHOHOHO2

! NIST / JANAF 1998

! enthalpy from Ruscic et al., J. Phys. Chem. A, 2006, 110 (21), 6592-6601

! (blank comment line)

1 1 1

0.0 2

35 'HAR' 'GHZ'

1 vib 26.92 0 1

2 vib 45.45 0 1

3 vib 71.3 0 1

4 vib 117.51 0 1

5 vib 134.17 0 1

6 vib 160.48 0 1

7 vib 168.5 0 1

8 vib 322.43 0 1

9 vib 381.12 0 1

10 vib 416.41 0 1

11 vib 505.85 0 1

12 vib 604.37 0 1

| | | | | |
|----|-----|-------------|---|---|
| 13 | vib | 650.94 0 | 1 | |
| 14 | vib | 687.08 0 | 1 | |
| 15 | vib | 811.73 0 | 1 | |
| 16 | vib | 912.83 0 | 1 | |
| 17 | vib | 1082.47 | 0 | 1 |
| 18 | vib | 1085.09 | 0 | 1 |
| 19 | vib | 1205.04 | 0 | 1 |
| 20 | vib | 1225.17 | 0 | 1 |
| 21 | vib | 1249.78 | 0 | 1 |
| 22 | vib | 1307.96 | 0 | 1 |
| 23 | vib | 1371.11 | 0 | 1 |
| 24 | vib | 1380.19 | 0 | 1 |
| 25 | vib | 1403.64 | 0 | 1 |
| 26 | vib | 1431.95 | 0 | 1 |
| 27 | vib | 1482.36 | 0 | 1 |
| 28 | vib | 1853.69 | 0 | 1 |
| 29 | vib | 3132.49 | 0 | 1 |
| 30 | vib | 3198.1 0 | 1 | |
| 31 | vib | 3637.2 0 | 1 | |
| 32 | vib | 3828.38 | 0 | 1 |
| 33 | vib | 3844.93 | 0 | 1 |
| 34 | qro | 3.73068 | 1 | 1 |
| 35 | qro | 0.851640294 | 1 | 2 |

trans-CHOHOH-FA+O2→ trans2-CHOH(OO)OH-FA(Ke)

KCAL MCC

13 ! Nt number of temperatures

200. 210. 220. 230. 240. 250. 260. 270. 280. 290. 300. 310. 320

3

reac trans-CHOHOH-FA_____ 0.0

CHOHOHHCOOH

! NIST / JANAF 1998

! enthalpy from Ruscic et al., J. Phys. Chem. A, 2006, 110 (21), 6592-6601

! (blank comment line)

1 1 1

0.0 2

29 'HAR' 'GHZ'

1 vib 50.86 0 1

2 vib 116.28 0 1

3 vib 131.78 0 1

4 vib 180.27 0 1

5 vib 200.65 0 1

6 vib 225.89 0 1

7 vib 344.54 0 1

8 vib 557.96 0 1

9 vib 702.85 0 1

10 vib 740.57 0 1

11 vib 899.54 0 1

12 vib 945.57 0 1

13 vib 1066.04 0 1

14 vib 1089.53 0 1

| | | | | |
|----|-----|-------------|---|---|
| 15 | vib | 1182.93 | 0 | 1 |
| 16 | vib | 1262.99 | 0 | 1 |
| 17 | vib | 1267.46 | 0 | 1 |
| 18 | vib | 1405.74 | 0 | 1 |
| 19 | vib | 1423.85 | 0 | 1 |
| 20 | vib | 1437.7 0 | 1 | |
| 21 | vib | 1451.48 | 0 | 1 |
| 22 | vib | 1822.7 0 | 1 | |
| 23 | vib | 3126.02 | 0 | 1 |
| 24 | vib | 3148.89 | 0 | 1 |
| 25 | vib | 3420.76 | 0 | 1 |
| 26 | vib | 3550.88 | 0 | 1 |
| 27 | vib | 3909.13 | 0 | 1 |
| 28 | qro | 5.71111 | 1 | 1 |
| 29 | qro | 1.842542397 | 1 | 2 |

reac O2_____ 0.0

O2

! NIST / JANAF 1998

! (blank comment line)

! (blank comment line)

2 1 4

0.0 3

7882.39 2

13120.9 1

32664.1 1

2 'HAR' 'GHZ'

1 vib 1778.6 0 1

2 qro 44.798983 1 2

prod tInt2FA_____ -39.2

HCOOHCHOHOHO2

! NIST / JANAF 1998

! enthalpy from Ruscic et al., J. Phys. Chem. A, 2006, 110 (21), 6592-6601

! (blank comment line)

1 1 1

0.0 2

35 'HAR' 'GHZ'

| | | | | |
|----|-----|----------|---|---|
| 1 | vib | 34.19 0 | 1 | |
| 2 | vib | 51.9 0 | 1 | |
| 3 | vib | 121.28 0 | 1 | |
| 4 | vib | 138.68 0 | 1 | |
| 5 | vib | 175.87 0 | 1 | |
| 6 | vib | 195.71 0 | 1 | |
| 7 | vib | 228.89 0 | 1 | |
| 8 | vib | 356.01 0 | 1 | |
| 9 | vib | 473.44 0 | 1 | |
| 10 | vib | 504.47 0 | 1 | |
| 11 | vib | 610.08 0 | 1 | |
| 12 | vib | 657.08 0 | 1 | |
| 13 | vib | 705.91 0 | 1 | |
| 14 | vib | 776.25 0 | 1 | |
| 15 | vib | 882.24 0 | 1 | |
| 16 | vib | 903.4 0 | 1 | |
| 17 | vib | 1067.15 | 0 | 1 |
| 18 | vib | 1089.23 | 0 | 1 |
| 19 | vib | 1233.91 | 0 | 1 |
| 20 | vib | 1270.9 0 | 1 | |
| 21 | vib | 1287.55 | 0 | 1 |

| | | | | |
|----|-----|-------------|---|---|
| 22 | vib | 1307.18 | 0 | 1 |
| 23 | vib | 1361.02 | 0 | 1 |
| 24 | vib | 1409.24 | 0 | 1 |
| 25 | vib | 1445 0 | 1 | |
| 26 | vib | 1480.99 | 0 | 1 |
| 27 | vib | 1488.16 | 0 | 1 |
| 28 | vib | 1823.26 | 0 | 1 |
| 29 | vib | 3142.24 | 0 | 1 |
| 30 | vib | 3157.84 | 0 | 1 |
| 31 | vib | 3431.97 | 0 | 1 |
| 32 | vib | 3509.07 | 0 | 1 |
| 33 | vib | 3800.34 | 0 | 1 |
| 34 | qro | 3.1495 1 | 1 | |
| 35 | qro | 1.089529724 | 1 | 2 |

Polyrate/GaussRate Input files for O₂ + •CHOHOH (+FA)

Cis-Int0-FA→ Cis-Post0-FA

*General

TITLE

HOCHOH + O2 +(FA)-> OHCHO + HO2

Calculation of first reactant (CH4)

END

ATOMS

1 C

2 H

3 O

4 O

5 H

6 O

7 O

8 H

9 C

10 H

11 O

12 O

13 H

END

NOSUPERMOL

INPUNIT AU

DL ISPE

*OPTIMIZATION

OPTMIN OHOOK

OPTTS OHOOK

*SECOND

HESSCAL HHOOK

*REACT1

STATUS 6

Geometry in a.u.

GEOM

| | | | |
|----|-------------|-------------|-------------|
| 1 | -2.87574294 | -1.47343618 | 0.01754098 |
| 2 | -4.55096053 | -2.66254455 | -0.09660225 |
| 3 | -4.00947483 | 1.07987290 | -0.41984180 |
| 4 | -2.34533485 | 2.85313152 | -0.34602343 |
| 5 | -0.11467168 | -0.98199573 | 2.27862287 |
| 6 | -1.83164846 | -1.62937443 | 2.31420830 |
| 7 | -1.11897603 | -1.89357322 | -1.83918864 |
| 8 | -1.92540342 | -1.96693243 | -3.46622394 |
| 9 | 4.14396403 | 0.45335354 | -0.64572832 |
| 10 | 3.63523083 | 1.04377766 | -2.57037281 |
| 11 | 5.92762369 | -0.80766439 | -0.14835996 |
| 12 | 2.54179559 | 1.31267996 | 1.13081644 |
| 13 | 1.12347293 | 2.19078648 | 0.35793168 |

END

Energy in a.u.

ENERGY -530.447230450386

Frequencies in a.u.

VIB

| | | | |
|------------------|------------------|------------------|------------------|
| 0.1771483982E-01 | 0.1694863515E-01 | 0.1671092925E-01 | 0.1441709352E-01 |
| 0.1396370009E-01 | 0.8714004553E-02 | 0.6720286542E-02 | 0.6577570359E-02 |
| 0.6488737126E-02 | 0.6393672974E-02 | 0.6106418145E-02 | 0.5846227461E-02 |
| 0.5757646587E-02 | 0.5461900550E-02 | 0.5263190274E-02 | 0.4988081290E-02 |
| 0.4825270233E-02 | 0.3779683636E-02 | 0.3725576940E-02 | 0.3445947459E-02 |
| 0.3156497901E-02 | 0.2690659817E-02 | 0.2357733407E-02 | 0.2210758851E-02 |
| 0.1578516892E-02 | 0.1544815926E-02 | 0.8669992199E-03 | 0.8035234039E-03 |
| 0.7220515389E-03 | 0.6431899874E-03 | 0.5454608591E-03 | 0.2465796918E-03 |
| 0.2099245798E-03 | | | |

END

ELEC

2 0.0

END

SPECIES NONLINRP

end of react1 section

*PROD1

STATUS 6

Geometry in a.u.

GEOM

| | | | |
|----|-------------|-------------|-------------|
| 1 | 2.30365011 | 1.98972278 | 1.08620212 |
| 2 | 3.85333893 | 2.41009047 | 2.38557592 |
| 3 | 5.88773682 | -1.15152362 | -0.49882268 |
| 4 | 4.55964297 | -3.19018852 | -0.20293315 |
| 5 | 2.92202709 | -2.62146221 | 0.46350712 |
| 6 | 0.93432621 | 0.18653665 | 1.33285295 |
| 7 | 1.95566461 | 3.62070572 | -0.76578052 |
| 8 | 3.21780135 | 4.93184684 | -0.74895250 |
| 9 | -5.35134321 | -0.53919188 | 0.46278336 |
| 10 | -4.45902398 | -0.72253500 | 2.33483866 |
| 11 | -7.56256656 | -0.75221882 | 0.12336398 |
| 12 | -3.70978725 | -0.05702070 | -1.38676153 |
| 13 | -2.01908897 | 0.05647247 | -0.68992124 |

END

Energy in a.u.

ENERGY -530.442983653047

Frequencies in a.u.

VIB

| | | | |
|------------------|------------------|------------------|------------------|
| 0.1760762611E-01 | 0.1699653866E-01 | 0.1608182312E-01 | 0.1429533314E-01 |
| 0.1382637484E-01 | 0.8692700030E-02 | 0.8325066164E-02 | 0.6969662629E-02 |
| 0.6564025501E-02 | 0.6540578210E-02 | 0.6249210976E-02 | 0.6009400006E-02 |
| 0.5975089440E-02 | 0.5424536119E-02 | 0.5419221168E-02 | 0.4905122156E-02 |
| 0.4868878886E-02 | 0.3494328238E-02 | 0.3169537054E-02 | 0.3130150264E-02 |
| 0.2572479326E-02 | 0.2294980835E-02 | 0.1351326882E-02 | 0.1266864472E-02 |
| 0.9634969408E-03 | 0.7410741975E-03 | 0.5691487420E-03 | 0.5519151295E-03 |
| 0.3047018528E-03 | 0.2829692093E-03 | 0.2378578464E-03 | 0.1736917494E-03 |
| 0.1311236506E-03 | | | |

END

ELEC

2 0.0

END

SPECIES NONLINRP

*START

STATUS 4

Geometry in a.u.

GEOM

| | | | |
|---|------------|-------------|-------------|
| 1 | 2.55162087 | 1.14317300 | 1.10450883 |
| 2 | 3.31595651 | 1.57655146 | 2.96724589 |
| 3 | 5.37256625 | -0.48620367 | -0.04094489 |
| 4 | 4.53013012 | -2.64038753 | -0.67650136 |
| 5 | 2.37825362 | -2.24977358 | -0.05532381 |
| 6 | 0.98191042 | -0.66240741 | 0.83454822 |

| | | | |
|----|-------------|-------------|-------------|
| 7 | 2.30802761 | 3.08704546 | -0.47932545 |
| 8 | 3.37997854 | 4.47536678 | 0.00099758 |
| 9 | -5.28929505 | -0.52277176 | 0.40815609 |
| 10 | -4.25458496 | -1.47217206 | 1.94435603 |
| 11 | -7.53248690 | -0.40642699 | 0.31756450 |
| 12 | -3.78177926 | 0.48459400 | -1.34068529 |
| 13 | -2.03364463 | 0.18295213 | -0.88190514 |

END

Energy in a.u.

ENERGY -530.426202101295

HESSIAN

| | | | |
|-------------------|-------------------|-------------------|-------------------|
| 0.3550098096E+00 | | | |
| 0.2465725100E+00 | 0.6706311450E+00 | | |
| 0.2081983932E+00 | 0.2215523803E-02 | 0.6566125779E+00 | |
| -0.8164577779E-01 | -0.2335129612E-01 | -0.8851330012E-01 | 0.9009329732E-01 |
| -0.2681222823E-01 | -0.6298739675E-01 | -0.5069598332E-01 | 0.2926332509E-01 |
| 0.7701468813E-01 | | | |
| -0.9619881134E-01 | -0.4288456003E-01 | -0.2817257395E+00 | 0.1036827065E+00 |
| 0.4844870177E-01 | 0.2971685269E+00 | | |
| 0.3411437367E-01 | -0.4986025053E-01 | -0.1876003117E-01 | -0.5424291114E-02 |
| 0.6538107237E-02 | 0.5135408590E-02 | 0.2159706278E+00 | |
| -0.2521419808E-01 | -0.1482063285E-01 | 0.9816201219E-02 | 0.8069464889E-02 |
| -0.3614005525E-02 | -0.5498843168E-02 | 0.2045214508E+00 | 0.5020479707E+00 |
| -0.1515934940E-01 | 0.6442297635E-02 | -0.3621183005E-01 | 0.1575123549E-01 |
| -0.1009896619E-01 | -0.4772496818E-02 | 0.3629448649E-01 | 0.1354660038E+00 |
| 0.8179195017E-01 | | | |
| -0.5892865613E-01 | -0.3412824638E-02 | 0.1449871411E-01 | 0.3263882986E-02 |
| -0.4189535251E-04 | -0.3103989403E-03 | -0.1154864140E+00 | -0.2063301455E+00 |
| -0.5871717958E-01 | 0.2193330812E+00 | | |
| 0.5015099297E-02 | -0.1416139943E-01 | -0.2938436075E-01 | 0.5972879580E-02 |
| -0.1563193347E-02 | -0.8629766221E-03 | -0.1259883655E+00 | -0.4538981125E+00 |
| -0.1404816854E+00 | 0.1117989339E+00 | 0.5279250152E+00 | |
| 0.1560698970E-01 | -0.5942782011E-02 | 0.5495021499E-03 | 0.4110323405E-03 |
| 0.2935253383E-03 | -0.9013907494E-03 | -0.2677789245E-01 | -0.1235916111E+00 |
| -0.6247860993E-01 | 0.2300511582E-02 | 0.1672753519E+00 | 0.9606514761E-01 |
| 0.9087975303E-01 | 0.1774952979E-01 | -0.1205458148E-01 | -0.9038657725E-02 |
| -0.7948266457E-03 | 0.4668256811E-03 | -0.6739752365E-01 | -0.1410146000E-01 |
| 0.1353245706E-01 | -0.2030873113E-02 | -0.6681933602E-02 | -0.9001443354E-02 |
| 0.4372340699E-01 | | | |
| -0.5100228883E-01 | -0.5176455097E-01 | -0.5759911089E-02 | 0.3848387998E-02 |
| -0.2441159579E-03 | -0.2724496804E-03 | -0.1823091108E-01 | -0.2480349856E-01 |
| -0.1109170202E-01 | -0.1229903009E-01 | -0.2608472146E-01 | 0.5155382565E-02 |
| 0.6306075127E-01 | 0.1007600817E+00 | | |
| -0.3787612190E-01 | -0.2475286354E-01 | -0.1344244411E-02 | 0.2338283080E-02 |
| -0.1670380268E-02 | -0.5593233363E-03 | 0.9046475713E-02 | -0.1221941556E-01 |
| 0.7192248940E-02 | -0.9412119478E-02 | 0.5006006215E-02 | -0.2930410491E-01 |
| 0.2302776273E-01 | 0.6526695153E-02 | 0.4099665427E-01 | |

| | | | |
|-------------------|-------------------|-------------------|-------------------|
| -0.2491761676E+00 | -0.1817926399E+00 | -0.5586372721E-01 | -0.7616866852E-02 |
| -0.1956905853E-01 | -0.3772716621E-02 | -0.5694794857E-01 | 0.1553955977E-01 |
| 0.1761864176E-01 | -0.5221904054E-01 | 0.6252507042E-02 | 0.1618497938E-01 |
| -0.4171790468E-01 | 0.6707768076E-02 | 0.7014700917E-02 | 0.4031376875E+00 |
| -0.1357032010E+00 | -0.2973008536E+00 | -0.6179150057E-01 | -0.2547343260E-01 |
| -0.8273871129E-02 | -0.3255778267E-02 | -0.3935375224E-01 | 0.9633520425E-02 |
| 0.1147190276E-01 | 0.1080076362E+00 | -0.1999555507E-01 | -0.3454137398E-01 |
| -0.5680253458E-01 | 0.5439652601E-03 | 0.1959129174E-01 | 0.1916021564E+00 |
| 0.3921909444E+00 | | | |
| -0.3411673861E-01 | -0.4430916872E-01 | -0.1221148036E+00 | -0.2400496741E-01 |
| -0.2300097867E-01 | 0.8125081430E-02 | 0.2683266566E-03 | 0.4151739686E-03 |
| 0.8633702288E-02 | 0.5246133606E-01 | -0.1435929497E-01 | -0.7802009627E-02 |
| -0.1760425822E-01 | 0.7458489188E-02 | -0.1498372976E-01 | 0.5894707982E-02 |
| 0.4271310329E-01 | 0.1106025328E+00 | | |
| -0.8590099365E-01 | -0.5734731939E-02 | -0.4600933722E-01 | 0.1018949345E-01 |
| 0.8859302582E-02 | -0.8457519535E-02 | -0.3436691297E-02 | 0.1639565207E-01 |
| -0.9075982054E-02 | 0.4564329395E-02 | 0.3231268932E-02 | 0.1160426346E-02 |
| -0.1131700376E-01 | 0.5826026799E-02 | 0.4494259045E-02 | 0.8200019215E-02 |
| -0.4369636256E-01 | 0.2126594272E-01 | 0.2738144055E+00 | |
| 0.1164599185E-01 | -0.2020416942E+00 | 0.1514089508E+00 | 0.1018378989E-02 |
| -0.2097058827E-02 | 0.4535602608E-02 | 0.2243443722E-01 | -0.1332589571E-01 |
| 0.8547548987E-02 | 0.1193538322E-02 | -0.1393331780E-01 | -0.8946416699E-02 |
| -0.2281077596E-02 | 0.1383010060E-02 | 0.6438544038E-02 | -0.2222466279E-01 |
| -0.7140553114E-01 | 0.2442950106E-01 | 0.2270721416E+00 | 0.6122582871E+00 |
| -0.5649008469E-01 | 0.8994339358E-01 | -0.2243224461E+00 | -0.1022583969E-01 |
| 0.3641631164E-01 | -0.1672097889E-01 | -0.6480260622E-02 | -0.4378144251E-02 |
| 0.6870293133E-02 | -0.1404923560E-02 | 0.1272233536E-01 | 0.3925704429E-02 |
| 0.1711359769E-02 | -0.3468447601E-02 | -0.2690891902E-02 | 0.1664946637E-01 |
| 0.1661521280E-01 | 0.2214998870E-01 | 0.1460586008E+00 | -0.7047266724E-01 |
| 0.2845620273E+00 | | | |
| 0.2649556696E-02 | 0.6154129053E-02 | -0.5525197707E-03 | -0.3810728179E-03 |
| 0.2002192652E-02 | -0.7006563519E-03 | -0.2748438646E-02 | 0.1222164247E-02 |
| 0.2343924554E-03 | 0.1796040237E-03 | 0.7514415083E-03 | 0.4666867270E-03 |
| -0.4009838377E-03 | -0.2721602545E-03 | 0.2835988677E-03 | 0.3173998999E-02 |
| -0.1810925531E-02 | -0.1185173920E-02 | -0.1962391634E+00 | -0.2414367824E+00 |
| -0.8868189705E-01 | 0.1935033902E+00 | | |
| -0.2311879787E-01 | -0.3145064333E-01 | -0.1357430727E-01 | 0.9304780509E-03 |
| 0.2326524638E-02 | -0.1706999075E-03 | 0.5938956041E-03 | -0.1032627297E-02 |
| -0.5754964945E-03 | 0.6259473633E-03 | 0.2020513634E-02 | 0.6758283835E-03 |
| -0.1204578799E-02 | 0.1751990808E-03 | 0.5585288708E-03 | 0.1488609840E-02 |
| -0.1099738671E-02 | 0.5728535172E-02 | -0.2124643603E+00 | -0.3098059655E+00 |
| -0.7817242764E-01 | 0.2334634873E+00 | 0.3393058001E+00 | |
| 0.1985390894E-01 | 0.2323773454E-01 | 0.7889198679E-02 | 0.4788897470E-03 |
| 0.1306066503E-03 | -0.6835487499E-03 | 0.1657707811E-04 | -0.1712492661E-03 |
| -0.6772790516E-03 | -0.3103700511E-03 | 0.5849401354E-03 | 0.3629705063E-03 |
| 0.5983666805E-03 | 0.2874993746E-03 | -0.7120299174E-03 | -0.1075735761E-02 |
| 0.7470699466E-02 | -0.8867820709E-03 | -0.1096848951E+00 | -0.1172088276E+00 |

| | | | |
|-------------------|-------------------|-------------------|-------------------|
| -0.7290735989E-01 | 0.9007677726E-01 | 0.8553261445E-01 | 0.6785839838E-01 |
| -0.7733576258E-02 | -0.5106129246E-02 | -0.2652423703E-03 | 0.5304127777E-03 |
| 0.5651566479E-03 | 0.2064515605E-03 | 0.2964016103E-02 | -0.3118055494E-03 |
| -0.7425326188E-03 | 0.1758626927E-02 | -0.8963020955E-03 | -0.6247791742E-03 |
| -0.3470722736E-02 | 0.2661307907E-02 | 0.1341769447E-02 | 0.1015959718E-01 |
| 0.1208660052E-02 | 0.2265985243E-02 | 0.1500335026E-02 | 0.1758712774E-02 |
| -0.6243037357E-03 | -0.1471307617E-03 | -0.7230088180E-03 | 0.1567701555E-03 |
| 0.1115594790E+01 | | | |
| -0.1770178222E-02 | 0.4896901097E-03 | -0.7551973209E-03 | 0.1637744855E-03 |
| 0.2044179358E-03 | 0.9382891492E-04 | 0.4419188287E-03 | 0.6403921872E-04 |
| -0.4164699048E-04 | 0.4821554252E-03 | -0.3706199033E-03 | -0.2548223467E-03 |
| -0.4752449134E-03 | 0.9247596274E-03 | 0.5253671593E-04 | 0.3538643076E-02 |
| -0.1702892768E-02 | 0.2903434713E-02 | 0.5684889399E-03 | -0.5632153357E-03 |
| 0.5057814480E-03 | -0.1312368759E-03 | -0.1484199097E-03 | 0.3784786814E-04 |
| -0.6056626937E-01 | 0.3195595908E+00 | | |
| 0.2959794057E-02 | 0.3450328922E-04 | 0.1441719402E-02 | -0.3388474443E-03 |
| -0.4014649930E-03 | -0.1904031601E-03 | -0.8126244466E-03 | 0.3429895665E-03 |
| 0.2061435650E-03 | -0.5824219850E-03 | 0.2740170215E-03 | 0.1946335520E-04 |
| 0.9238833682E-03 | -0.1288666378E-02 | 0.5285013133E-04 | -0.6364823885E-02 |
| 0.2351795056E-02 | -0.5147207482E-02 | -0.9836370720E-03 | 0.4405118703E-03 |
| -0.4137463362E-03 | -0.5446024100E-05 | 0.3641410811E-03 | -0.3291629356E-04 |
| 0.6006615789E-01 | -0.1966281686E+00 | 0.5250237867E+00 | |
| -0.4658974297E-03 | -0.6507117366E-03 | -0.5221012975E-05 | 0.4741504690E-04 |
| 0.3630906337E-04 | 0.6411340051E-05 | 0.1844747582E-03 | -0.1004810178E-04 |
| -0.5584565479E-04 | 0.1370876925E-03 | -0.2954767518E-04 | -0.1759306453E-04 |
| -0.2062105764E-03 | 0.2252787365E-03 | 0.1507908946E-03 | 0.2548923355E-03 |
| 0.2946636362E-03 | 0.2294528739E-04 | 0.3296170334E-04 | 0.2101053273E-03 |
| -0.1043765119E-03 | 0.5184759582E-05 | -0.1337346040E-04 | -0.1911017321E-04 |
| -0.1045261431E+00 | 0.5149925337E-01 | -0.8426970343E-01 | 0.1316577891E+00 |
| -0.4313946735E-03 | -0.4606288856E-03 | 0.2368162277E-03 | -0.1234211728E-04 |
| -0.7676836969E-05 | -0.1318985571E-04 | 0.2197811090E-03 | -0.2610490486E-04 |
| -0.7866013934E-04 | 0.1159490350E-03 | -0.8767684926E-04 | -0.1625996902E-03 |
| -0.1532571283E-03 | 0.1888702999E-03 | 0.1223030289E-03 | 0.2404113817E-03 |
| 0.1532660146E-03 | -0.5037926632E-03 | 0.3825594267E-04 | 0.1655125614E-03 |
| -0.1141530259E-04 | -0.2308702892E-04 | -0.8041983548E-05 | 0.2769513915E-04 |
| 0.4787438133E-01 | -0.1150570961E+00 | 0.7563916264E-01 | -0.5771231513E-01 |
| 0.9156821500E-01 | | | |
| 0.4646160410E-03 | 0.9629398797E-03 | -0.2520348609E-03 | -0.2964619075E-04 |
| -0.3562821919E-04 | 0.1113029459E-04 | -0.2763623968E-03 | 0.4108454498E-04 |
| 0.6236374912E-04 | -0.1149092331E-03 | -0.2272423698E-04 | 0.2929885680E-04 |
| 0.3303679762E-03 | -0.5339131519E-04 | -0.1592607992E-03 | -0.3515886757E-03 |
| -0.7954408000E-03 | 0.4942658533E-03 | 0.4297414966E-05 | -0.4523179319E-03 |
| 0.2281903843E-03 | 0.9781286254E-05 | 0.2677814734E-04 | -0.6532229013E-05 |
| -0.7800093958E-01 | 0.7534281878E-01 | -0.1897148290E+00 | 0.9113332902E-01 |
| -0.1079489381E+00 | 0.2002787259E+00 | | |
| 0.5313704246E-02 | 0.3970479003E-02 | 0.1431053822E-03 | -0.3545754563E-03 |
| -0.3946023813E-03 | -0.1515146926E-03 | -0.2049640878E-02 | 0.2194047963E-03 |

| | | | |
|-------------------|-------------------|-------------------|-------------------|
| 0.5192411349E-03 | -0.1205983724E-02 | 0.5535886207E-03 | 0.4528405983E-03 |
| 0.2361160990E-02 | -0.1809041757E-02 | -0.9933143938E-03 | -0.7572383114E-02 |
| -0.9146212600E-03 | -0.1833582407E-02 | -0.9837803978E-03 | -0.1491495422E-02 |
| 0.5319800955E-03 | 0.8864561808E-04 | 0.5065641666E-03 | -0.1293867378E-03 |
| -0.8236099186E+00 | 0.6164279756E-01 | -0.6878724643E-01 | -0.3638729447E-01 |
| 0.7517481130E-02 | -0.9835577295E-02 | 0.9463415659E+00 | |
| -0.8342981497E-05 | -0.7084739687E-03 | 0.1315467789E-03 | -0.9318226051E-05 |
| -0.4923245732E-04 | -0.1614145852E-04 | -0.8284799316E-04 | 0.1495317092E-03 |
| 0.5801287796E-04 | 0.1365802883E-03 | -0.1079057761E-03 | -0.4878729262E-04 |
| -0.1526190884E-03 | -0.7481250537E-04 | 0.8593332489E-04 | -0.3394034325E-03 |
| 0.5937957618E-03 | -0.7260274485E-03 | -0.7472103270E-04 | 0.4656531305E-03 |
| -0.2517772669E-03 | -0.2586405054E-04 | -0.1184869540E-03 | -0.5394780636E-04 |
| 0.5593596479E-01 | -0.8858882095E-01 | 0.2210264242E-01 | 0.1859203109E-01 |
| 0.1856437046E-01 | 0.7273635787E-02 | -0.4236872572E-01 | 0.4931131710E-01 |
| -0.2047126404E-03 | 0.3406871285E-03 | -0.4586825712E-03 | 0.6439109539E-04 |
| 0.8450180369E-04 | 0.6999228842E-04 | -0.2126456909E-04 | 0.1598389355E-03 |
| 0.1441566495E-03 | -0.6245071629E-05 | -0.2545503993E-03 | 0.3735921228E-04 |
| 0.5988818418E-04 | 0.1355826589E-03 | -0.1393820805E-03 | 0.1164232416E-02 |
| -0.8973509663E-03 | 0.1342137028E-02 | 0.1678296088E-03 | -0.2822109681E-03 |
| 0.2819631632E-03 | 0.5544326580E-04 | -0.2208253831E-04 | -0.5902455238E-04 |
| -0.5964431989E-01 | 0.2195135502E-01 | -0.1078319541E+00 | -0.2810278075E-01 |
| 0.7646404966E-02 | 0.1175111607E-01 | 0.2905217160E-01 | -0.3094054299E-01 |
| 0.8009957160E-01 | | | |
| 0.6795727231E-02 | 0.6575708233E-02 | -0.3603780249E-03 | -0.5928124956E-03 |
| -0.8239109166E-03 | -0.2087457530E-03 | -0.2388738139E-02 | 0.3581704392E-03 |
| 0.7415030467E-03 | -0.1715077678E-02 | 0.6599027511E-03 | 0.6220474875E-03 |
| 0.2757946974E-02 | -0.2873976402E-02 | -0.1662459869E-02 | -0.1570755541E-01 |
| 0.7896896608E-03 | -0.6301610556E-02 | -0.1291485660E-02 | -0.1855524065E-02 |
| 0.8124352837E-03 | 0.7685791117E-05 | 0.5951920507E-03 | -0.7532445652E-04 |
| -0.1551060288E+00 | -0.5548920915E-01 | 0.9697117725E-01 | 0.6816631629E-02 |
| 0.8235463870E-03 | -0.8046630823E-03 | -0.8877320318E-01 | -0.3006497798E-01 |
| 0.5496556973E-01 | 0.6855032246E+00 | | |
| 0.2294326886E-02 | -0.3148232296E-02 | 0.1932510258E-02 | 0.4535891966E-04 |
| 0.7978308985E-04 | -0.1144161668E-03 | -0.5646314115E-03 | -0.3651160038E-04 |
| 0.5986064279E-04 | -0.3248211781E-03 | 0.7697072261E-03 | 0.4746617045E-03 |
| 0.1160631027E-04 | -0.7946624556E-03 | -0.4318971521E-03 | 0.4069183921E-03 |
| 0.4067778769E-02 | -0.2828711277E-03 | -0.1046567382E-02 | 0.1469959752E-02 |
| -0.1096386430E-02 | 0.7634300055E-04 | 0.7653097602E-04 | -0.1418681094E-03 |
| -0.2315590805E-01 | -0.1150868198E+00 | 0.1067270421E+00 | -0.1197230634E-01 |
| 0.6495872753E-02 | 0.2526234278E-01 | -0.2403941175E-01 | 0.1723145053E-01 |
| -0.4473428707E-02 | -0.6021339411E-02 | 0.1274764076E+00 | |
| -0.1015718245E-02 | 0.1400546556E-02 | -0.1808626427E-02 | 0.2875282530E-03 |
| 0.9806423726E-04 | 0.1658980071E-03 | 0.2478279332E-04 | 0.1226710696E-04 |
| 0.1731937341E-03 | 0.4290208094E-05 | -0.1975045284E-03 | 0.1257471458E-03 |
| -0.7412176856E-03 | 0.3260207055E-03 | -0.8207832489E-03 | -0.1120279680E-02 |
| -0.4490345710E-03 | 0.3285623746E-02 | 0.5687985493E-03 | -0.2898307425E-03 |
| 0.7250696335E-03 | 0.5206882786E-04 | -0.3002496411E-03 | 0.3141634883E-04 |

| | | | |
|-------------------|-------------------|-------------------|-------------------|
| 0.4303203555E-01 | 0.1077542012E+00 | -0.2348493981E+00 | 0.2055691790E-01 |
| 0.2463090506E-01 | -0.2072106763E-01 | 0.4465094989E-01 | -0.4215394288E-02 |
| 0.1898306905E-01 | -0.8255189079E-02 | -0.1660143053E+00 | 0.3104578613E+00 |
| -0.1091185554E-01 | -0.1111377192E-01 | -0.4558742773E-03 | 0.9295526727E-03 |
| 0.1172128786E-02 | 0.3025596026E-03 | 0.2646193899E-02 | -0.3582097672E-03 |
| -0.9410681355E-03 | 0.2349432933E-02 | -0.6394727149E-03 | -0.7838061223E-03 |
| -0.4142387916E-02 | 0.4157887622E-02 | 0.2246374948E-02 | 0.6031671560E-02 |
| 0.1852023830E-02 | 0.2867087166E-02 | 0.8675738977E-03 | 0.3956236226E-02 |
| -0.1752156505E-02 | 0.3087233639E-03 | -0.6800551306E-03 | 0.1135323950E-03 |
| -0.3791425739E-01 | 0.9510685533E-04 | 0.1223738165E-02 | 0.2449108527E-02 |
| 0.1502589763E-02 | -0.2528705284E-02 | 0.6831703077E-02 | -0.1537755668E-02 |
| 0.2449797023E-02 | -0.4363063149E+00 | 0.6429043201E-01 | -0.9804496728E-01 |
| 0.4668608558E+00 | | | |
| -0.1467298092E-02 | 0.7723671134E-02 | -0.3780288823E-02 | -0.4656589360E-03 |
| -0.7888629623E-03 | 0.1092186653E-04 | -0.6688319645E-03 | -0.3376730343E-03 |
| 0.3225305118E-03 | 0.4797618893E-04 | -0.5127338602E-03 | -0.3863568159E-03 |
| 0.1825644983E-02 | -0.2095241429E-03 | 0.6927174393E-03 | -0.1850809319E-02 |
| -0.7404828224E-02 | -0.4661037873E-03 | 0.1025606399E-02 | -0.2569744065E-02 |
| 0.1648230915E-02 | 0.3029836853E-04 | -0.2406447366E-03 | 0.2662551356E-03 |
| -0.1924476037E-01 | 0.2753870644E-03 | -0.9958505168E-02 | -0.4693387829E-03 |
| -0.1488881568E-02 | 0.3988407002E-03 | -0.3392416981E-02 | 0.3331613918E-02 |
| 0.6551796055E-02 | 0.8732672840E-01 | -0.3860126460E-01 | 0.3724431417E-01 |
| -0.6269713989E-01 | 0.4082348507E-01 | | |
| -0.6022165089E-02 | -0.6688252102E-02 | 0.1745409504E-02 | 0.9853438556E-04 |
| 0.4316902301E-03 | 0.1325234200E-04 | 0.2342378328E-02 | -0.3942958836E-03 |
| -0.9338363770E-03 | 0.1593715942E-02 | -0.2995537047E-03 | -0.6290780493E-03 |
| -0.1249410712E-02 | 0.2044898441E-02 | 0.2471997028E-02 | 0.4022143005E-02 |
| 0.1516474037E-02 | -0.3698799270E-02 | 0.4912164355E-03 | 0.1851611753E-02 |
| -0.1687813541E-02 | -0.5305557436E-04 | -0.7116261303E-04 | -0.1765111585E-03 |
| 0.3283294753E-01 | -0.1096196945E-01 | 0.1143649126E-01 | 0.7042361576E-03 |
| 0.4153087001E-03 | -0.2001366605E-02 | 0.6380333255E-02 | 0.6600847355E-02 |
| -0.4220321775E-02 | -0.1364443620E+00 | 0.3809875543E-01 | -0.7574800352E-01 |
| 0.9530348831E-01 | -0.3254435220E-01 | 0.7342858015E-01 | |

END

ELEC
2 0.0
END

SPECIES NONLINTS

*PATH

SCALEMASS 1.000000
SSTEP 0.05
INH 1
NSTEPS 99999

CURV dgrad
RPM pagem
SIGN product

SRANGE
slp 1.50
slm -1.50
END

PRPATH
xmol
END

*TUNNELING

ZCT
SCT

*RATE

PRDELG
FORWARDK
TST
CVT

TEMP
200.
210.
220.
230.
240.
250.
260.
270.
280.
290.
300.
310.
320
END

Trans-Int1-FA→ Tran-Post₁-FA

*General

TITLE

HOCHOH + O2 -> OHCHO + HO2
Calculation of first reactant (CH4)
END

ATOMS

1 C
2 H
3 O
4 O
5 H
6 O
7 O
8 H
9 C
10 H
11 O
12 O
13 H

END

NOSUPERMOL

INPUNIT AU

DL ISPE

*OPTIMIZATION

OPTMIN OHOOK
OPTTS OHOOK

*SECOND

HESSCAL HHOOK

*REACT1

STATUS 6

Geometry in a.u.

GEOM

| | | | |
|---|-------------|-------------|-------------|
| 1 | -1.68104010 | 0.31538161 | 0.37319975 |
| 2 | -0.53962612 | -1.36434776 | 0.69653851 |
| 3 | -3.49581986 | -0.33259502 | -1.63942226 |
| 4 | -5.22607722 | -1.81053857 | -0.75840336 |
| 5 | -4.22312498 | -0.07436075 | 2.87399986 |
| 6 | -2.97480291 | 1.17761443 | 2.42504522 |

| | | | |
|----|-------------|-------------|-------------|
| 7 | -0.19465000 | 2.18451730 | -0.58806714 |
| 8 | -1.10659370 | 3.76084978 | -0.49152122 |
| 9 | 5.38809261 | -0.93956102 | 0.12227717 |
| 10 | 7.38745054 | -1.46912618 | 0.15872005 |
| 11 | 3.70903024 | -2.29564008 | 0.80477039 |
| 12 | 5.09762839 | 1.37864741 | -0.77105760 |
| 13 | 3.29893118 | 1.78593762 | -0.77128780 |

END

Energy in a.u.

ENERGY -530.453709766726

Frequencies in a.u.

VIB

| | | | |
|------------------|------------------|------------------|------------------|
| 0.1751881806E-01 | 0.1744342154E-01 | 0.1657229088E-01 | 0.1457160693E-01 |
| 0.1427266921E-01 | 0.8446035649E-02 | 0.6754118804E-02 | 0.6524458174E-02 |
| 0.6395438814E-02 | 0.6288613097E-02 | 0.6247264216E-02 | 0.5959515167E-02 |
| 0.5694407995E-02 | 0.5582270202E-02 | 0.5490573500E-02 | 0.4944038091E-02 |
| 0.4932114897E-02 | 0.4159160706E-02 | 0.3698513439E-02 | 0.3130555323E-02 |
| 0.2965913403E-02 | 0.2753692769E-02 | 0.2304802652E-02 | 0.1897278947E-02 |
| 0.1736502978E-02 | 0.1469095563E-02 | 0.7677164272E-03 | 0.7312045515E-03 |
| 0.6113311561E-03 | 0.5354050617E-03 | 0.3248596974E-03 | 0.2070685383E-03 |
| 0.1226541297E-03 | | | |

END

ELEC

2 0.0

END

SPECIES NONLINRP

*PROD1

STATUS 6

Geometry in a.u.

GEOM

| | | | |
|----|-------------|-------------|-------------|
| 1 | -0.32867854 | 2.01012681 | 0.00233723 |
| 2 | 1.52230531 | 2.90903647 | 0.14230903 |
| 3 | -7.59679244 | -1.60857083 | 0.51250279 |
| 4 | -5.47024911 | -0.85479943 | -0.47793928 |
| 5 | -5.30139047 | 0.97198571 | -0.21603519 |
| 6 | -2.31892178 | 3.08850263 | -0.04103267 |
| 7 | -0.08224940 | -0.50623035 | -0.11869025 |
| 8 | -1.73919936 | -1.29593146 | -0.23814639 |
| 9 | 6.37775449 | -0.60796145 | 0.07006662 |
| 10 | 8.38148252 | -1.11867030 | 0.09288936 |
| 11 | 5.61213974 | 1.52018013 | 0.16191721 |
| 12 | 4.93731018 | -2.65005709 | -0.07148472 |

```

13      3.17580382   -2.11686132   -0.09197543
END
# Energy in a.u.
ENERGY  -530.453941571102
# Frequencies in a.u.
VIB
0.1686052418E-01  0.1675917703E-01  0.1629431483E-01  0.1455349014E-01
0.1429824402E-01  0.8445966798E-02  0.8422652460E-02  0.6644443869E-02
0.6538325647E-02  0.6484980405E-02  0.6297632004E-02  0.6083803178E-02
0.5844468922E-02  0.5574643184E-02  0.5376958285E-02  0.5040777674E-02
0.4947966048E-02  0.3597058099E-02  0.3373073019E-02  0.3158709158E-02
0.3086735125E-02  0.2098575789E-02  0.1148909162E-02  0.8292213600E-03
0.7773456600E-03  0.7180441860E-03  0.6960300412E-03  0.6027305452E-03
0.5181955037E-03  0.2935647779E-03  0.2254098193E-03  0.1963405414E-03
0.1234948463E-03
END

ELEC
2  0.0
END

SPECIES  NONLINRP

# end of react1 section

*START

STATUS 4

# Geometry in a.u.
GEOM
1      1.88856913   -1.26848902    0.89049810
2      0.76577136   -0.94854130    2.57488092
3      1.33370418    1.91541609   -0.47891651
4      3.57154816    2.71453765   -0.82801696
5      4.62389494    0.86051593    0.01410737
6      4.28104178   -1.21850782    0.86759650
7      0.66878671   -2.77504853   -0.76665377
8      1.86838860   -3.28999899   -2.04366644
9      -4.68915545    0.67021738    0.31717219
10     -6.39651348    1.82632171    0.15199879
11     -3.46985880    0.47220045    2.21177571
12     -4.17290880   -0.47098449   -1.85264725
13     -2.62644582   -1.44416332   -1.63652872
END
# Energy in a.u.
ENERGY  -530.437256957006

```

HESSIAN

```

0.8047973491E+00
0.8989491173E-01 0.2521355730E+00
-0.1664653468E+00 0.1785958439E+00 0.6300193241E+00
-0.1350640462E+00 0.2607035725E-01 0.1371180521E+00 0.1516719538E+00
0.2007192887E-01 -0.4859649268E-01 -0.3778400164E-01 -0.2145467961E-01
0.5847826123E-01
0.1281842700E+00 -0.4677157116E-01 -0.2575150146E+00 -0.1372027071E+00
0.5157710243E-01 0.2691278206E+00
-0.2567112430E-01 -0.3187890669E-01 0.6804408859E-02 0.2002429369E-02
-0.1333592639E-02 0.1573427768E-02 0.5948416896E+00
-0.6415130471E-02 0.4605926307E-01 -0.2430460688E-01 0.9232409392E-03
-0.1176816229E-01 0.6842448870E-02 0.1299356988E+00 0.1360287559E+00
0.6962439823E-02 -0.2348829980E-01 -0.3129452249E-01 -0.3157222862E-02
0.1765851722E-01 -0.5169017306E-02 -0.5248633000E-01 -0.4600664237E-01
0.5628430474E-01
-0.3602449217E-01 0.1864457180E-01 0.5053822852E-02 0.3494909889E-02
-0.5723663713E-02 0.1674667552E-02 -0.4904654866E+00 -0.1966397532E+00
0.8522681512E-01 0.5215604601E+00
0.2565937702E-01 -0.3785059049E-01 0.3337482181E-01 0.6827457231E-03
-0.1508424928E-02 -0.6393972767E-04 -0.1179492018E+00 -0.9880305125E-01
0.3480110669E-01 0.1566955919E+00 0.2340545268E+00
-0.1297159983E-01 0.1883170567E-01 -0.2060185823E-03 0.1055795741E-04
-0.6439662785E-03 -0.5055333073E-03 0.4972243948E-01 0.3576038971E-01
-0.3645097669E-01 -0.6786326778E-01 -0.8912416269E-01 0.7109127696E-01
-0.1227586615E-01 -0.3312455887E-01 0.1148734658E-01 -0.2257995461E-02
0.1357309986E-02 -0.5592690317E-03 -0.5805594683E-01 0.2204793480E-01
-0.1082996970E-01 -0.2213341932E-01 -0.9169020259E-02 0.4203596240E-02
0.1361198836E+00
-0.1040933386E+00 0.4277432810E-01 -0.2125566126E-01 0.5150656526E-02
-0.6096749741E-02 0.2478634659E-02 0.2027361466E-01 -0.3237829352E-01
0.2104778180E-01 -0.1649872812E-01 0.1179411073E-02 -0.1561840279E-01
0.2461252202E-01 0.6957902967E-02
0.4704281349E-01 -0.1603658062E-01 0.6390201336E-02 -0.5472215587E-03
0.2727111162E-02 -0.7376861381E-03 -0.7170074927E-02 0.1896785442E-01
0.4873124816E-02 0.4459293871E-02 -0.1316036332E-01 -0.2618652685E-01
-0.8141588796E-02 0.1725244892E-01 0.3468313268E-01
-0.4725062451E+00 -0.3567852860E-01 0.5363950403E-01 -0.2747402734E-01
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| -0.2488366628E-03 | 0.1463884242E-01 | -0.5373342043E-02 | 0.9067550949E-02 |
| 0.4745886565E-02 | -0.2087010001E-01 | 0.4394665193E-01 | -0.1118106699E-01 |
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| -0.1729400092E-03 | -0.3984002653E-03 | -0.5060952500E-03 | 0.2370615312E-03 |
| 0.8532817700E-04 | 0.5135004098E-03 | -0.1630159560E-04 | -0.8664379546E-03 |
| -0.1173267426E-02 | -0.9537405553E-03 | -0.3192045150E-02 | -0.8235491279E-03 |
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| 0.1247662807E-02 | 0.7501652786E-02 | 0.1369517156E-01 | -0.3438923841E-02 |
| 0.8226852488E-03 | -0.1367804581E-02 | -0.1475434382E-03 | -0.1721242768E-02 |
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| -0.3056431512E-04 | 0.8019495123E-04 | 0.1953719168E-03 | -0.7176820313E-04 |
| 0.8158539879E-04 | -0.1161961173E-03 | -0.1918955138E-03 | 0.1206950577E-03 |
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| 0.3340160046E-02 | 0.4970881674E-02 | 0.6120312490E-02 | -0.6112945856E-03 |
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| 0.1522781484E-02 | -0.6014385536E-03 | -0.5299576635E-02 | -0.4593251596E-02 |
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| 0.2571320587E-01 | -0.1637115193E-01 | -0.1063548920E-01 | 0.2175541148E-02 |
| 0.3272889178E-02 | -0.3513052697E-02 | -0.2678123560E-02 | -0.1374943524E-02 |
| 0.8538088553E-02 | 0.1856252647E+00 | -0.1429970825E+00 | 0.1611349211E-01 |
| -0.2087818840E+00 | 0.1597394670E+00 | | |
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| -0.6323387946E-04 | -0.5066558732E-03 | -0.7374757703E-03 | -0.2995044311E-03 |
| -0.1537398319E-03 | 0.4705810066E-03 | 0.4450003200E-03 | -0.3353796141E-03 |
| -0.5448992446E-04 | -0.3238360262E-03 | 0.2855107912E-03 | 0.8164076819E-03 |
| 0.3245412894E-03 | -0.2381114905E-03 | -0.4062907984E-04 | -0.7962960857E-03 |
| -0.5639561502E-02 | 0.2374238861E-02 | -0.4518386049E-03 | 0.2085260411E-02 |
| 0.4374216149E-01 | -0.2886678405E-01 | 0.8727116622E-02 | 0.2448378695E-03 |
| -0.3895465100E-02 | -0.4132074089E-02 | -0.4880632465E-02 | 0.5698311228E-02 |
| -0.3832448592E-03 | -0.7452942072E-01 | 0.3751096069E-01 | -0.5903001046E-01 |
| 0.3590685182E-01 | -0.8820742310E-02 | 0.5958883592E-01 | |

END

ELEC

2 0.0

END

SPECIES NONLINTS

*PATH

SCALEMASS 1.000000

SSTEP 0.1

INH 1

NSTEPS 99999

CURV dgrad

RPM pagem

SIGN product

SRANGE

slp 1.50

slm -1.50

END

PRPATH

```

    xmol
  END

*TUNNELING

  ZCT
  SCT

*RATE

  PRDELG
  FORWARDK
  TST
  CVT

  TEMP
    200.
    210.
    220.
    230.
    240.
    250.
    260.
    270.
    280.
    290.
    300.
    310.
    320
  END

Trans-Int2-FA→ Tran-Post2-FA

*General

  TITLE
  HOCHOH + O2 -> OHCHO + HO2
  Calculation of first reactant (CH4)
  END

  ATOMS
    1  C
    2  H
    3  O
    4  O
    5  H

```

6 O
7 O
8 H
9 C
10 H
11 O
12 O
13 H
END

NOSUPERMOL

INPUNIT AU

DL ISPE

*OPTIMIZATION

OPTMIN OHOOK
OPTTS OHOOK

*SECOND

HESSCAL HHOOK

*REACT1

STATUS 6

Geometry in a.u.

GEOM

| | | | |
|----|-------------|-------------|-------------|
| 1 | 2.33426354 | 0.84178961 | 1.14659800 |
| 2 | 4.03231802 | 1.18708172 | 2.25787024 |
| 3 | 3.24135794 | 0.36506691 | -1.46076441 |
| 4 | 4.40242177 | -1.77652164 | -1.58173677 |
| 5 | 2.15405223 | -2.74221767 | 1.58281622 |
| 6 | 1.06571766 | -1.31541415 | 1.93283960 |
| 7 | 0.85425860 | 2.87050295 | 1.10154927 |
| 8 | -0.71463726 | 2.50877107 | 0.17715215 |
| 9 | -4.75755388 | -0.24725428 | -0.72889185 |
| 10 | -6.67459059 | -0.57400460 | -1.42687160 |
| 11 | -3.56940100 | 1.63144158 | -1.22102548 |
| 12 | -3.96083568 | -2.13076313 | 0.67549004 |
| 13 | -2.21685713 | -1.81364359 | 1.22226641 |

END

Energy in a.u.

ENERGY -530.462064869693

Frequencies in a.u.

VIB

| | | | |
|------------------|------------------|------------------|------------------|
| 0.1731562542E-01 | 0.1598852985E-01 | 0.1563719715E-01 | 0.1438817750E-01 |
| 0.1431710124E-01 | 0.8307386471E-02 | 0.6780542143E-02 | 0.6747861442E-02 |
| 0.6583906220E-02 | 0.6420986632E-02 | 0.6201262282E-02 | 0.5955969482E-02 |
| 0.5866527873E-02 | 0.5790654647E-02 | 0.5622129295E-02 | 0.4962916508E-02 |
| 0.4862279154E-02 | 0.4116190877E-02 | 0.4019766545E-02 | 0.3536849086E-02 |
| 0.3216381876E-02 | 0.2993878900E-02 | 0.2779729002E-02 | 0.2298540349E-02 |
| 0.2157159591E-02 | 0.1622094786E-02 | 0.1042883454E-02 | 0.8917369844E-03 |
| 0.8013042143E-03 | 0.6318602694E-03 | 0.5525862440E-03 | 0.2364975567E-03 |
| 0.1557945415E-03 | | | |

END

ELEC

2 0.0

END

SPECIES NONLINRP

*PROD1

STATUS 6

Geometry in a.u.

GEOM

| | | | |
|----|-------------|-------------|-------------|
| 1 | 0.99515169 | 2.03624691 | 0.00000198 |
| 2 | 2.81480678 | 3.00494509 | -0.00000558 |
| 3 | 6.55938982 | 0.24142849 | -0.00005282 |
| 4 | 5.69704353 | -2.06499737 | 0.00004922 |
| 5 | 3.84876098 | -1.85801756 | 0.00003222 |
| 6 | 0.87656948 | -0.27436658 | 0.00000387 |
| 7 | -0.93132206 | 3.53440478 | 0.00001143 |
| 8 | -2.56148675 | 2.56869237 | 0.00002088 |
| 9 | -5.34448642 | -1.31660157 | -0.00000936 |
| 10 | -7.17673087 | -2.26963770 | -0.00002070 |
| 11 | -5.16584872 | 0.96490637 | 0.00000954 |
| 12 | -3.46352673 | -2.90742405 | -0.00001692 |
| 13 | -1.83362849 | -1.98332341 | -0.00000747 |

END

Energy in a.u.

ENERGY -530.471536812023

Frequencies in a.u.

VIB

| | | | |
|------------------|------------------|------------------|------------------|
| 0.1569395185E-01 | 0.1496797874E-01 | 0.1452644021E-01 | 0.1435021331E-01 |
| 0.1393129066E-01 | 0.8277616101E-02 | 0.7818470481E-02 | 0.7116264531E-02 |
| 0.6810522567E-02 | 0.6635354452E-02 | 0.6560018890E-02 | 0.6500607716E-02 |
| 0.6017346720E-02 | 0.5925361899E-02 | 0.5884679150E-02 | 0.5146429259E-02 |

| | | | |
|------------------|------------------|------------------|------------------|
| 0.4989565601E-02 | 0.4721887617E-02 | 0.4405312908E-02 | 0.3399910855E-02 |
| 0.3229004691E-02 | 0.2913808831E-02 | 0.1329234907E-02 | 0.1167746804E-02 |
| 0.1078009157E-02 | 0.9108134131E-03 | 0.8009016205E-03 | 0.7133818374E-03 |
| 0.5883735741E-03 | 0.4449772340E-03 | 0.3386412599E-03 | 0.3312238206E-03 |
| 0.1677195784E-03 | | | |

END

ELEC

2 0.0

END

SPECIES NONLINRP

*START

STATUS 4

Geometry in a.u.

GEOM

| | | | |
|----|-------------|-------------|-------------|
| 1 | 2.05353122 | 1.10453901 | 1.43548373 |
| 2 | 3.54194618 | 1.67937754 | 2.72763778 |
| 3 | 4.24108082 | 0.19862415 | -1.11343844 |
| 4 | 3.83924837 | -2.15564052 | -1.40481298 |
| 5 | 2.21261404 | -2.28837495 | 0.24306520 |
| 6 | 1.01747060 | -1.10031227 | 1.72167522 |
| 7 | 0.76451698 | 3.00540555 | 0.53342092 |
| 8 | -0.78463095 | 2.42039875 | -0.33979435 |
| 9 | -4.79172418 | -0.30410342 | -0.64925988 |
| 10 | -6.74803953 | -0.67188780 | -1.20229001 |
| 11 | -3.59791491 | 1.45672313 | -1.47696969 |
| 12 | -3.96142218 | -1.97385700 | 0.97358645 |
| 13 | -2.16864399 | -1.63881909 | 1.37546767 |

END

Energy in a.u.

ENERGY -530.449754588743

HESSIAN

| | | | |
|-------------------|-------------------|-------------------|------------------|
| 0.5636739881E+00 | | | |
| 0.7645835017E-01 | 0.7300644610E+00 | | |
| 0.3078242766E+00 | -0.3989832272E-01 | 0.3991475443E+00 | |
| -0.1943889588E+00 | -0.5346949001E-01 | -0.1296128064E+00 | 0.2148396876E+00 |
| -0.6177902537E-01 | -0.7170301624E-01 | -0.4864338665E-01 | 0.5808884335E-01 |
| 0.9000453740E-01 | | | |
| -0.1393138881E+00 | -0.4376582203E-01 | -0.1618713264E+00 | 0.1436819249E+00 |
| 0.4650366341E-01 | 0.1675568740E+00 | | |
| 0.1073301148E-01 | -0.2873060772E-01 | -0.4570853183E-01 | 0.2046858246E-02 |
| 0.1778153593E-02 | 0.2676584305E-02 | 0.1001808869E+00 | |
| -0.5293177303E-02 | -0.3070828399E-01 | 0.8540890714E-02 | 0.3706795134E-02 |

| | | | |
|-------------------|-------------------|-------------------|-------------------|
| -0.1988989627E-03 | -0.6559092543E-02 | 0.1282807730E+00 | 0.5984458169E+00 |
| -0.4405695031E-01 | 0.2032100282E-01 | -0.3172416541E-02 | 0.1459786999E-01 |
| -0.7376056425E-02 | -0.1717751658E-01 | -0.3336056141E-01 | 0.3950672731E-01 |
| 0.8473237359E-01 | | | |
| -0.2478627553E-01 | -0.1131896978E-01 | 0.3351432180E-01 | 0.6434520056E-03 |
| 0.7345603418E-03 | -0.8335735838E-03 | -0.4858559956E-01 | -0.1197913989E+00 |
| -0.5913353997E-02 | 0.1121124324E+00 | | |
| -0.1702978737E-01 | -0.8833327670E-02 | -0.1228281276E-01 | 0.4956229192E-02 |
| 0.1816390347E-03 | -0.4564869866E-02 | -0.6190134379E-01 | -0.5294825510E+00 |
| -0.9205872035E-01 | 0.6693672315E-01 | 0.5758784681E+00 | |
| 0.3109588476E-01 | 0.7338778901E-02 | -0.2199425010E-01 | -0.1426586597E-02 |
| -0.1383127884E-03 | -0.1001470268E-03 | 0.1307025570E-01 | -0.3324818623E-01 |
| -0.4243776438E-01 | -0.6307496394E-01 | 0.9780199215E-01 | 0.1245070309E+00 |
| 0.5277740133E-01 | 0.3078858421E-01 | -0.3968745056E-01 | -0.5347098655E-02 |
| -0.2728222465E-02 | 0.3453815349E-02 | -0.2748077912E-01 | -0.2110881908E-01 |
| 0.3767562618E-01 | -0.8415757570E-02 | -0.9143020800E-04 | -0.2624930269E-01 |
| 0.3861166127E-01 | | | |
| -0.1284934764E-01 | -0.5217983697E-01 | 0.1879950246E-03 | 0.1084771318E-02 |
| -0.8287831593E-04 | -0.9014130784E-03 | -0.2255194811E-01 | -0.3591244965E-01 |
| 0.8523730114E-02 | -0.5648306265E-02 | -0.2606850918E-01 | 0.7370847552E-02 |
| 0.3514947237E-01 | 0.1326074679E+00 | | |
| -0.5571391566E-01 | -0.4738172285E-01 | 0.3449238168E-01 | 0.5137534461E-02 |
| 0.6711483441E-03 | -0.3896743112E-02 | 0.3270303141E-01 | 0.4061928849E-02 |
| -0.2022499673E-01 | -0.2356378905E-01 | 0.4709707529E-02 | -0.6883694014E-02 |
| 0.2111622183E-01 | -0.1105559567E-01 | 0.1956353321E-01 | |
| -0.1806069745E+00 | -0.1169044820E+00 | -0.5899155829E-02 | -0.3300531208E-02 |
| -0.2852684407E-01 | 0.4701321889E-02 | -0.2409866142E-01 | 0.2643544600E-02 |
| 0.2862780011E-01 | -0.3450862097E-01 | -0.7054881015E-02 | 0.4531940084E-01 |
| -0.3757948407E-01 | 0.1384811683E-02 | 0.9292898338E-02 | 0.2589192605E+00 |
| -0.9475687662E-01 | -0.3234879720E+00 | -0.1809351494E-01 | -0.1986347897E-01 |
| -0.1877616362E-01 | 0.8614995309E-02 | -0.3812684362E-01 | 0.9689604505E-03 |
| 0.3888399073E-01 | 0.6619120972E-01 | 0.3145774492E-02 | -0.6856963930E-01 |
| -0.4132208297E-01 | -0.2104594713E-01 | 0.3912827210E-01 | 0.1333490128E+00 |
| 0.4410595318E+00 | | | |
| 0.9529468345E-02 | 0.2524333038E-01 | -0.1043742376E+00 | -0.9866409075E-02 |
| -0.1565176585E-01 | 0.1504945822E-01 | 0.2066268901E-01 | 0.1805616928E-02 |
| -0.9419905918E-02 | 0.6344721210E-01 | -0.3205100820E-03 | -0.5547627742E-01 |
| -0.3141514800E-02 | -0.1426473050E-02 | -0.1762577555E-01 | -0.8317611443E-01 |
| -0.2884082546E-01 | 0.1580693523E+00 | | |
| -0.1960380585E+00 | 0.1061240167E+00 | -0.1087118540E+00 | -0.1771815782E-01 |
| 0.3096380942E-01 | -0.1348115628E-01 | -0.1700163752E-01 | 0.1089272021E-01 |
| 0.5987605448E-02 | 0.2061404388E-02 | 0.1664304012E-01 | 0.3725315348E-02 |
| -0.8952074444E-02 | 0.2025418563E-03 | 0.6968829838E-02 | 0.3704473886E-01 |
| -0.2297033003E-02 | 0.4078294097E-02 | 0.4943900785E+00 | |
| 0.8543893696E-01 | -0.2551053091E+00 | 0.8876882227E-01 | 0.3225123758E-02 |
| 0.3855877257E-02 | -0.9954773543E-03 | 0.2078956532E-01 | -0.3019063121E-02 |
| -0.7726492670E-02 | 0.2418959709E-02 | -0.1288238603E-01 | -0.9025677168E-02 |

| | | | |
|-------------------|-------------------|-------------------|-------------------|
| -0.2760510593E-02 | 0.1629550326E-02 | 0.9316228075E-02 | 0.1671368582E-01 |
| -0.7729036707E-01 | 0.2120070808E-01 | -0.3422594690E-01 | 0.4369453331E+00 |
| -0.8891946025E-01 | 0.7350982408E-01 | -0.1323781452E+00 | -0.1966556548E-01 |
| 0.2284897091E-01 | -0.1925497268E-02 | 0.7995501583E-02 | -0.1424346534E-01 |
| 0.8084779427E-02 | -0.4897800090E-02 | 0.8449920772E-02 | 0.4863028145E-02 |
| 0.6516190203E-02 | -0.3595637643E-02 | -0.8549955023E-02 | 0.3777126812E-02 |
| 0.3637051086E-01 | 0.1961152453E-01 | 0.2509628668E+00 | -0.5184254320E-01 |
| 0.2120555130E+00 | | | |
| -0.3202077369E-01 | 0.2635033063E-01 | -0.1722822436E-01 | 0.3821156697E-02 |
| -0.1570009694E-02 | -0.2201052679E-03 | 0.3432142792E-02 | 0.2664908029E-03 |
| -0.1852777688E-02 | -0.2335131827E-03 | -0.4335621408E-02 | -0.1602243354E-02 |
| 0.8273085632E-03 | 0.1065944268E-02 | 0.2184016597E-03 | -0.5240252085E-02 |
| -0.1280562889E-01 | 0.3456488891E-02 | -0.2599280947E+00 | -0.9156291705E-01 |
| -0.1350389051E+00 | 0.2745697875E+00 | | |
| 0.3568576386E-01 | 0.2161512877E-01 | 0.2149813721E-01 | 0.2651224319E-02 |
| -0.4087564271E-02 | 0.1974820552E-02 | 0.8207730231E-03 | 0.4653690774E-03 |
| 0.5807336259E-04 | -0.7037188258E-03 | -0.2783450269E-02 | -0.4310713392E-03 |
| 0.1928681439E-02 | -0.5604810381E-03 | -0.1025677881E-02 | -0.5390792682E-02 |
| -0.2506747985E-02 | -0.2022276472E-02 | -0.1145951230E+00 | -0.9840031970E-01 |
| -0.6335258079E-01 | 0.7202395207E-01 | 0.9316331269E-01 | |
| -0.2246118217E-01 | 0.1240506604E-01 | -0.1107830419E-01 | -0.2478529195E-02 |
| 0.1521942861E-02 | 0.2700131662E-02 | 0.1919368907E-02 | 0.2599556214E-03 |
| -0.8423377927E-05 | 0.8041511832E-03 | -0.2630944687E-02 | -0.2373787121E-02 |
| -0.9184575062E-03 | 0.6734461956E-03 | 0.2642176715E-02 | 0.1252446733E-02 |
| -0.9931064449E-02 | -0.2758245520E-02 | -0.1345631762E+00 | -0.4851656687E-01 |
| -0.9934060748E-01 | 0.1452011581E+00 | 0.3899270713E-01 | 0.1165204929E+00 |
| -0.4294081196E-02 | -0.9150171380E-03 | -0.6082553720E-03 | 0.2012228770E-03 |
| 0.1379452978E-03 | -0.8376788268E-04 | 0.5826573191E-03 | -0.7166170461E-04 |
| -0.4158060858E-03 | 0.5898007939E-03 | -0.3583232015E-03 | -0.5478870219E-03 |
| -0.1524506491E-02 | 0.8956792402E-03 | 0.8508248006E-03 | 0.1395037053E-02 |
| -0.1483239176E-02 | 0.1339481958E-02 | 0.9887575405E-04 | 0.2625850967E-03 |
| -0.1042954363E-02 | -0.2550608784E-02 | -0.5102428011E-02 | 0.3043679638E-02 |
| 0.8206788392E+00 | | | |
| -0.6088831882E-02 | 0.2431178215E-01 | -0.7423783528E-02 | 0.4772667921E-03 |
| -0.2131687211E-02 | 0.3562086041E-03 | -0.1772927948E-03 | -0.6914760686E-03 |
| 0.1096666158E-02 | -0.1097191095E-02 | -0.2114434849E-02 | 0.4849593700E-03 |
| 0.3087587647E-02 | -0.1848242008E-03 | -0.2808122334E-02 | -0.1578140363E-01 |
| -0.1397127327E-01 | 0.2713999737E-02 | 0.2042435995E-01 | -0.4965118813E-02 |
| 0.1147242493E-01 | -0.2717363705E-01 | -0.9025044013E-02 | -0.1022185762E-01 |
| 0.2419741615E+00 | 0.7192287202E+00 | | |
| 0.1662810779E-02 | -0.1700509370E-01 | 0.5779039661E-02 | -0.3452273421E-03 |
| 0.1558355623E-02 | -0.3517796699E-03 | 0.6403812307E-03 | 0.4645160756E-03 |
| -0.1225286576E-02 | 0.1226663618E-02 | 0.9065290263E-03 | -0.9132539502E-03 |
| -0.2844106572E-02 | 0.6338615154E-03 | 0.3137449602E-02 | 0.1251213190E-01 |
| 0.9330911597E-02 | -0.2653272323E-02 | -0.1470015600E-01 | 0.3070974096E-02 |
| -0.9807616209E-02 | 0.1892098271E-01 | 0.4724450958E-02 | 0.1066377397E-01 |
| 0.7587209930E-01 | -0.2837213366E+00 | 0.4541870606E+00 | |

| | | | |
|-------------------|-------------------|-------------------|-------------------|
| 0.6225675414E-03 | -0.4848829538E-03 | -0.1369029981E-03 | -0.8882978472E-04 |
| 0.5751544505E-04 | -0.3690539672E-04 | -0.2396487619E-03 | 0.1968672119E-05 |
| 0.1054334377E-03 | -0.8746532580E-04 | 0.1970839453E-03 | 0.1866266361E-03 |
| 0.1866311370E-03 | -0.1935339802E-03 | -0.2865781523E-03 | -0.7742432137E-03 |
| 0.2097412484E-03 | 0.2218612287E-03 | -0.1488071049E-02 | 0.9493594847E-04 |
| -0.6045955650E-03 | 0.2217601539E-02 | 0.6099593587E-03 | 0.5431320814E-03 |
| -0.2912072836E+00 | -0.3454117599E-01 | -0.6849835643E-01 | 0.3175848710E+00 |
| 0.3577268982E-03 | -0.1531817724E-02 | 0.5125085865E-03 | -0.8711162856E-04 |
| 0.1643075592E-03 | -0.1054959622E-04 | 0.4262029608E-04 | 0.5467647314E-04 |
| -0.6652089342E-04 | 0.9357026214E-04 | 0.1515752876E-03 | -0.2081565682E-04 |
| -0.8191293815E-04 | 0.4934487956E-04 | 0.2073534215E-03 | 0.1266594436E-02 |
| 0.8622162623E-03 | -0.4699810300E-03 | -0.1677675619E-02 | -0.9101034037E-04 |
| -0.1399805811E-02 | 0.2082140285E-02 | 0.1392858073E-02 | 0.2004012758E-02 |
| -0.4086106815E-01 | -0.6369973356E-01 | -0.2125080498E-01 | 0.5308364967E-01 |
| 0.6538591766E-01 | | | |
| -0.3538018146E-03 | 0.1844637181E-02 | -0.3779170760E-03 | -0.5871739563E-05 |
| -0.1973089354E-03 | 0.5608949553E-04 | -0.3968264300E-05 | 0.2633741632E-04 |
| 0.5419949507E-04 | -0.5102092546E-04 | -0.1169016451E-03 | 0.4834917871E-04 |
| 0.2530458701E-03 | -0.7376248276E-04 | -0.1661514552E-03 | -0.1575765438E-02 |
| -0.1221587320E-02 | -0.1974202027E-03 | 0.1918283393E-02 | -0.4495684684E-03 |
| 0.6014439967E-03 | -0.2425478315E-02 | -0.4310509421E-04 | -0.7607775621E-04 |
| -0.6378280806E-01 | -0.1868860372E-01 | -0.8188863217E-01 | 0.8312121374E-01 |
| -0.5341217177E-02 | 0.6709587410E-01 | | |
| 0.7020957458E-02 | -0.1949289025E-01 | 0.4277841113E-02 | -0.1253380070E-02 |
| 0.2011017609E-02 | -0.4855177094E-03 | -0.1224674337E-02 | -0.1076617518E-04 |
| 0.3531293713E-03 | -0.8879396685E-07 | 0.2263705383E-02 | 0.6355154223E-03 |
| -0.1589622323E-03 | -0.8880564216E-03 | 0.1981998334E-03 | 0.5641394241E-02 |
| 0.9249355937E-02 | -0.1902582629E-02 | -0.3247184255E-01 | -0.3304520901E-02 |
| -0.1819663663E-01 | 0.1390082157E-01 | 0.1232629257E-01 | 0.7065787286E-02 |
| -0.3241708446E+00 | -0.2602054900E+00 | 0.9141131852E-01 | -0.1613072117E-01 |
| -0.3888862020E-01 | 0.1372271673E-01 | 0.3076042631E+00 | |
| 0.3134572096E-02 | -0.2032635239E-01 | 0.3599226658E-02 | -0.6278180425E-03 |
| 0.1908338150E-02 | -0.5498975375E-03 | -0.5305812695E-03 | 0.1391986842E-03 |
| -0.3332539982E-03 | 0.6492897351E-03 | 0.2130824466E-02 | 0.1494405555E-04 |
| -0.1873483113E-02 | 0.1069851172E-04 | 0.1364948474E-02 | 0.9862067356E-02 |
| 0.9013812731E-02 | -0.1097064130E-03 | -0.2526262580E-01 | 0.6557587540E-02 |
| -0.1292995530E-01 | 0.2436487990E-01 | -0.2763806557E-03 | 0.9327800006E-02 |
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| -0.6646299022E-02 | 0.1254926527E-01 | 0.3120819783E+00 | 0.5301233061E+00 |
| 0.2157627495E-02 | -0.3272594573E-03 | -0.1549399790E-02 | -0.3145594244E-04 |
| -0.5000323710E-04 | -0.2935167911E-03 | -0.8687282924E-03 | -0.4637069415E-03 |
| 0.8469912526E-03 | -0.6159000167E-03 | 0.6653550335E-03 | 0.1054291965E-02 |
| 0.1097202174E-02 | -0.5378162352E-03 | -0.1930672140E-02 | -0.3827337593E-02 |
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| 0.2937440331E-02 | -0.1716014425E-02 | 0.9212477137E-03 | -0.1224774282E-01 |
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| 0.3814456682E-02 | 0.1769663785E-01 | -0.1166701205E+00 | -0.2428604607E+00 |

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| 0.1719411109E+00 | | | |
| -0.1704177908E-02 | 0.2041731612E-01 | -0.7140035833E-02 | -0.3158667938E-03 |
| -0.2202132862E-02 | 0.4484958849E-03 | -0.1618664718E-02 | -0.5467177888E-03 |
| 0.2161157046E-02 | -0.2009491373E-02 | -0.5781050979E-03 | 0.2083061036E-02 |
| 0.3764230074E-02 | -0.2620679310E-02 | -0.5066959719E-02 | -0.3354731621E-01 |
| -0.1642384679E-01 | 0.8711977699E-03 | 0.7856658705E-02 | -0.4845527906E-02 |
| 0.5271119635E-02 | -0.8522701395E-02 | -0.1435763727E-02 | -0.3540986555E-02 |
| -0.1833989438E+00 | 0.5265232654E-01 | -0.8739006676E-01 | -0.1358310906E-01 |
| 0.2630812372E-01 | -0.3106436597E-01 | 0.5067249490E-01 | -0.3869680377E-02 |
| 0.1166772750E-01 | 0.5461875654E+00 | | |
| 0.3541896849E-02 | -0.8721450456E-02 | 0.2473436880E-02 | -0.1225359269E-03 |
| 0.7988822752E-03 | -0.2170182515E-03 | -0.2835632364E-03 | 0.3607180917E-03 |
| -0.5507853109E-04 | 0.3931587743E-03 | 0.8016187825E-03 | 0.3534136994E-04 |
| -0.1854930665E-02 | -0.8704728996E-03 | 0.2957179464E-03 | 0.2769622063E-03 |
| 0.9222230115E-02 | -0.7453896823E-03 | -0.7732829400E-02 | 0.2523536129E-02 |
| -0.4257543178E-02 | 0.1112823858E-01 | 0.2654454929E-02 | 0.4212874683E-02 |
| 0.5005921351E-01 | -0.2067217995E+00 | 0.1276815487E+00 | 0.2939188787E-03 |
| 0.4353093854E-02 | 0.6064570092E-02 | -0.1022402554E-01 | -0.6403583191E-01 |
| 0.6724822540E-01 | 0.2449703000E-01 | 0.3229111916E+00 | |
| -0.8615950761E-03 | 0.1245844210E-01 | -0.4399858585E-02 | 0.2482661208E-03 |
| -0.9851234235E-03 | 0.1414741479E-03 | -0.1198695054E-02 | -0.2870287472E-03 |
| 0.1590113797E-02 | -0.6935253130E-03 | -0.6535896817E-03 | 0.8538570658E-03 |
| 0.1317148331E-02 | -0.1152918041E-02 | -0.3045918549E-02 | -0.1175686751E-01 |
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| 0.1685701097E-01 | -0.4540393653E-02 | 0.1626258353E-01 | 0.7041976869E-01 |
| -0.1522543197E-01 | 0.1680144142E+00 | -0.2030169925E+00 | 0.2696411954E+00 |
| -0.9886256818E-03 | -0.2882225798E-01 | 0.9116777722E-02 | 0.8604457079E-03 |
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| -0.3909172092E-02 | 0.3219722678E-02 | 0.3527103035E-03 | -0.3215076129E-02 |
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| 0.1003670241E-01 | -0.3637806778E+00 | -0.6997253402E-01 | -0.7235414516E-01 |
| 0.3684365187E+00 | | | |
| -0.6820200648E-02 | -0.3394005429E-02 | 0.7608032568E-03 | -0.1981928577E-04 |
| 0.6662694007E-04 | 0.1144523797E-03 | 0.5902952837E-03 | -0.4220168389E-03 |
| -0.7740676322E-03 | 0.1142113169E-02 | -0.1252410855E-03 | -0.1613160919E-02 |
| 0.8670663673E-03 | 0.2608337818E-02 | 0.2515813997E-02 | 0.8161724497E-02 |
| -0.7194054712E-02 | -0.1376727083E-02 | 0.5407454406E-03 | 0.2416897836E-03 |
| -0.1030120296E-02 | 0.1658375631E-03 | -0.1651135594E-02 | 0.1902628321E-02 |
| 0.3769109788E-01 | 0.1399992628E-01 | 0.7190165187E-02 | 0.3905555127E-03 |
| -0.4451294078E-03 | 0.5647244886E-02 | -0.4917980261E-02 | -0.4563865030E-02 |
| -0.3353431864E-02 | -0.9135234252E-01 | -0.6327617108E-01 | -0.7759678752E-02 |

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|-------------------|-------------------|-------------------|-------------------|
| 0.5356090700E-01 | 0.6415503835E-01 | | |
| -0.5892746238E-03 | -0.4742860768E-02 | 0.1776889877E-02 | -0.2331436456E-03 |
| -0.6212383374E-04 | 0.1124993234E-03 | 0.1472672709E-02 | 0.1355068872E-03 |
| -0.1642147463E-02 | 0.6515782190E-03 | 0.9484455701E-04 | -0.1147383293E-02 |
| 0.1411582199E-02 | 0.1353735796E-02 | 0.2488365371E-02 | 0.7521141749E-03 |
| 0.2287735365E-02 | -0.7759911054E-02 | -0.1341792446E-02 | 0.1044661196E-02 |
| -0.1697328942E-02 | 0.2587434818E-02 | 0.1604287450E-02 | 0.1399996002E-02 |
| -0.3792344854E-01 | 0.1972076821E-02 | -0.1143397549E-01 | -0.2252577572E-02 |
| 0.5164352725E-02 | 0.1693998188E-02 | 0.3327765613E-02 | -0.6908601748E-02 |
| -0.2739983141E-03 | -0.5631475825E-01 | 0.2803070337E-03 | -0.4951398897E-01 |
| 0.8845184734E-01 | -0.2223921481E-02 | 0.6599698476E-01 | |

END

ELEC

2 0.0

END

SPECIES NONLINTS

*PATH

SCALEMASS 1.000000

SSTEP 0.05

INH 1

NSTEPS 99999

CURV dgrad

RPM pagem

SIGN product

SRANGE

slp 1.50

slm -1.50

END

PRPATH

xmol

END

*TUNNELING

ZCT

SCT

*RATE

PRDELG

FORWARDK

TST
CVT

TEMP
200.
210.
220.
230.
240.
250.
260.
270.
280.
290.
300.
310.
320
END