Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for Detailed Kinetics of Hydrogen Abstraction from *trans*-Decalin by OH Radicals: The Role of Hindered Internal Rotation Treatment

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Text 1: Procedure of the hindered internal rotation (HIR) treatment

For the hindered internal rotation (HIR) treatment, the hindrance potentials, $V(\theta)$, as a function of torsional angle, θ, along the "single" bonds (i.e., C−H−O) were explicitly achieved at the M06-2X/cc-pVDZ level via relaxed surface scans with the step size of 10^{o} for dihedral angles with respect to the rotations (cf. Figure S4). The HIR parameters were automatically identified using the Graphical User Interface[1, 2] of the Multi-Species Multi-Channels (MSMC) code[3]. The detailed procedure of the HIR correction calculation can be found in our previous work[4].

Table S1: Optimized geometries, electronic energies at 0 K ($E_{elec}^{0\,K}$), zero-point energy (ZPE) corrections and harmonic wavenumbers of the species involved with the lowest-energy conformer of a given species, calculated at M06-2X/aug-cc-pVTZ level of theory for the title reaction.

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
OH	8	0.000000000	0.000000000	0.107999000	-75.733789	0.008530	3742.0378 (3737.8)[5]		
($C_{\infty v}$)	1	0.000000000	0.000000000	-0.863995000					
H_2O	8	0.000000000	0.000000000	0.116332000	-76.4300922	0.021565	1615.7190	3873.1681	3977.2474
(C_{2v})	1	0.000000000	0.762680000	-0.465326000			(1595.0; 3657.0[6]; 3756.0[5])		
	1	0.000000000	-0.762680000	-0.465326000					
***trans*-decalin**	6	0.231198000	1.447960000	1.265011000	-391.8812396	0.264561	128.2510	138.7097	225.2882
(C_{2h})	6	-0.232054000	0.730838000	0.000000000			295.4305	299.2017	349.6000
	6	0.232054000	-0.730838000	0.000000000			353.2302	403.7147	409.9897
	6	-0.231198000	-1.447960000	1.265011000			454.7298	496.5110	525.3609
	6	0.231198000	-0.727551000	2.528000000			561.7497	763.4679	808.9011
	6	-0.231198000	0.727551000	2.528000000			836.9552	856.9196	861.4395
	1	-1.331749000	0.719629000	0.000000000			871.3062	896.9392	921.2008
	1	1.326043000	1.498840000	1.257144000			933.6658	995.6808	1006.1007
	1	-0.130415000	2.478858000	1.257848000			1006.3011	1053.7625	1068.4028
	1	-1.326043000	-1.498840000	1.257144000			1072.5602	1072.8441	1111.5335
	1	0.130415000	-2.478858000	1.257848000			1122.1913	1162.0243	1164.2754
	1	-0.135876000	-1.243588000	3.416490000			1181.1728	1187.2287	1248.9036
	1	1.324497000	-0.755077000	2.574838000			1256.4514	1277.3193	1282.3113
	1	-1.324497000	0.755077000	2.574838000			1302.7185	1312.1073	1326.6001
	1	0.135876000	1.243588000	3.416490000			1334.5982	1364.6456	1366.8607
	1	1.331749000	-0.719629000	0.000000000			1372.7374	1376.3114	1384.6417
	6	-0.231198000	-1.447960000	-1.265011000			1385.5693	1389.5915	1396.8925
	6	0.231198000	1.447960000	-1.265011000			1402.4054	1478.5277	1484.4597
	6	-0.231198000	0.727551000	-2.528000000			1485.7245	1486.5942	1488.9092
	6	0.231198000	-0.727551000	-2.528000000			1493.4688	1501.8388	1505.4999
	1	0.130415000	-2.478858000	-1.257848000			2980.4444	2991.0765	3019.0236
	1	-0.135876000	-1.243588000	-3.416490000			3019.6927	3023.8801	3025.2572
	1	-1.326043000	-1.498840000	-1.257144000			3030.1142	3030.9267	3035.1380
	1	1.324497000	-0.755077000	-2.574838000			3035.7281	3070.3914	3071.0927
	1	1.326043000	1.498840000	-1.257144000			3075.8162	3076.2994	3082.8438

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	-0.130415000	2.478858000	-1.257848000			3083.3511	3087.2574	3087.9770
	1	-1.324497000	0.755077000	-2.574838000					
	1	0.135876000	1.243588000	-3.416490000					
RC	6	1.228063000	1.559371000	0.201587000	-467.6195182	0.274989	25.9564	51.5949	89.5614
(C_1)	6	-0.026187000	0.693372000	0.259542000			105.3752	133.3222	148.8797
	6	-0.038574000	-0.341179000	-0.871133000			236.2434	298.7938	305.3710
	6	1.241177000	-1.173422000	-0.869466000			307.0486	354.1714	359.5320
	6	2.493711000	-0.303501000	-0.919020000			407.9646	412.4631	461.3821
	6	2.499788000	0.716468000	0.216704000			502.2192	530.8142	566.7120
	1	-0.008845000	0.134437000	1.210187000			767.7201	816.6001	843.2678
	1	1.201161000	2.152695000	-0.719439000			859.4947	861.9240	878.1512
	1	1.226728000	2.268194000	1.032498000			900.5751	925.5259	936.3288
	1	1.254387000	-1.786792000	0.039474000			997.6375	1007.0414	1010.6425
	1	1.227106000	-1.871602000	-1.709342000			1055.7740	1074.1458	1077.2177
	1	3.390512000	-0.923698000	-0.880568000			1079.8706	1112.6709	1125.3966
	1	2.519989000	0.230755000	-1.873647000			1162.9958	1167.2155	1185.1118
	1	2.568043000	0.189138000	1.175765000			1187.3190	1250.0988	1256.6072
	1	3.382408000	1.354267000	0.152589000			1278.8161	1284.4628	1300.3537
	1	-0.076595000	0.219091000	-1.816765000			1312.1841	1326.7331	1339.3256
	6	-1.284839000	-1.218993000	-0.786327000			1363.6312	1366.3904	1370.0452
	6	-1.306102000	1.523974000	0.252718000			1375.0427	1383.3949	1384.4394
	6	-2.548015000	0.641432000	0.339892000			1388.1639	1398.7860	1400.9198
	6	-2.565383000	-0.388843000	-0.786739000			1480.1717	1485.4712	1488.6295
	1	-1.290059000	-1.931886000	-1.614148000			1489.2438	1491.5055	1494.2472
	1	-3.437280000	-1.037814000	-0.694158000			1503.3458	1506.4495	2931.6314
	1	-1.231648000	-1.803565000	0.138725000			2988.3837	3018.3318	3025.5940
	1	-2.657099000	0.130682000	-1.745916000			3026.8582	3032.3794	3034.4700
	1	-1.338221000	2.109178000	-0.673618000			3039.0224	3044.5166	3045.8290
	1	-1.285172000	2.239538000	1.077637000			3080.8390	3081.7030	3085.4729
	1	-2.544724000	0.119097000	1.301546000			3086.1068	3093.2978	3095.0722
	1	-3.451193000	1.252585000	0.311738000			3095.5189	3098.3854	3754.2902
	8	0.159533000	-1.481806000	2.583649000					
	1	1.112401000	-1.441922000	2.391705000					
TS1	6	-1.261676000	-1.138687000	-0.959511000	-467.6165521	0.272032	-420.1937	66.1743	72.1126
(C_1)	6	0.007253000	-0.589943000	-0.326623000			122.1450	129.7494	153.0679

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	6	0.009253000	0.935847000	-0.252494000			227.6269	294.2591	303.2389
	6	-1.260693000	1.457200000	0.414883000			340.5900	343.4264	405.4812
	6	-2.523761000	0.919690000	-0.250995000			410.1384	456.2349	491.2002
	6	-2.520592000	-0.606125000	-0.282191000			521.5338	549.0552	634.2324
	1	0.028582000	-0.961628000	0.753248000			757.9343	808.4750	837.6116
	1	-1.269390000	-0.847174000	-2.017025000			854.8883	861.2835	874.9085
	1	-1.241963000	-2.230011000	-0.933417000			900.6525	924.4589	930.6763
	1	-1.247333000	1.158283000	1.470166000			997.6845	1006.4311	1014.4099
	1	-1.257074000	2.549328000	0.406035000			1056.9606	1066.9460	1078.0560
	1	-3.411708000	1.288080000	0.264871000			1086.7128	1118.9447	1126.5500
	1	-2.575223000	1.297559000	-1.276799000			1160.9912	1170.0264	1181.7675
	1	-2.563488000	-0.990274000	0.742632000			1187.1908	1225.7159	1247.4063
	1	-3.410591000	-0.979518000	-0.790387000			1268.0928	1275.1306	1290.7967
	1	0.018023000	1.298849000	-1.291570000			1303.2727	1313.5065	1326.9156
	6	1.270276000	1.445821000	0.440973000			1353.8718	1363.9062	1367.2093
	6	1.279441000	-1.135217000	-0.958380000			1370.4556	1380.2223	1383.1180
	6	2.529378000	-0.614621000	-0.255024000			1385.4727	1391.0976	1396.1315
	6	2.538748000	0.911230000	-0.217558000			1472.6689	1480.6221	1481.6163
	1	1.269577000	2.538183000	0.444756000			1483.5899	1486.0811	1488.5442
	1	3.420196000	1.271157000	0.314963000			1497.0395	1499.2707	1714.4367
	1	1.243445000	1.119826000	1.486257000			2977.4072	3019.0565	3023.6018
	1	2.606146000	1.298024000	-1.239550000			3023.7475	3029.0087	3030.1837
	1	1.296165000	-0.830520000	-2.012353000			3034.1614	3036.7746	3042.7507
	1	1.255373000	-2.226771000	-0.944817000			3072.7334	3076.2145	3078.7591
	1	2.541096000	-0.997771000	0.769145000			3080.5917	3084.9942	3087.2988
	1	3.425507000	-0.990577000	-0.750390000			3088.0956	3092.5210	3760.5185
	8	0.033247000	-1.413303000	2.250549000					
	1	-0.799074000	-0.969782000	2.481363000					
TS2a (C_1)	6	-1.238306000	0.922179000	-0.791957000	-467.6143019	0.272082	-566.0915	51.7947	72.8060
	6	0.149157000	0.306944000	-0.731869000			92.1203	134.2363	144.8831
	6	0.230565000	-0.774690000	0.352247000			222.9557	301.6187	303.7321
	6	-0.870363000	-1.815257000	0.168140000			341.8028	353.4303	408.3364
	6	-2.257275000	-1.178919000	0.147963000			411.1269	458.6702	492.4749
	6	-2.353460000	-0.099046000	-0.927158000			527.8999	556.0957	706.1238
	1	0.324493000	-0.194924000	-1.696337000			773.3666	824.4095	839.1489

Species	Cartesian coordinate (Å)				$E_{elec}^{0\ K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	-1.403281000	1.509041000	0.185697000			859.5610	863.2696	882.2671
	1	-1.297217000	1.697704000	-1.558720000			897.0897	922.5266	937.3368
	1	-0.699656000	-2.340307000	-0.778369000			997.5882	1005.8166	1007.5018
	1	-0.805387000	-2.565933000	0.958911000			1055.2624	1066.1187	1076.8735
	1	-3.023580000	-1.938416000	-0.011053000			1078.5650	1111.8323	1124.9767
	1	-2.464681000	-0.730358000	1.125247000			1151.7987	1165.5402	1177.8783
	1	-2.273612000	-0.571183000	-1.912837000			1184.5439	1225.7075	1256.7498
	1	-3.324754000	0.394866000	-0.890279000			1267.0776	1269.7957	1295.7668
	1	0.072646000	-0.274412000	1.319292000			1305.5860	1325.1885	1330.2960
	6	1.621183000	-1.403169000	0.380900000			1349.5244	1363.4085	1367.5053
	6	1.238960000	1.358310000	-0.539212000			1370.4982	1380.0121	1381.9195
	6	2.628075000	0.727537000	-0.502316000			1387.5450	1396.1291	1401.4443
	6	2.711860000	-0.353126000	0.573224000			1419.7351	1477.9241	1484.0910
	1	1.669426000	-2.155691000	1.171179000			1489.7905	1491.1492	1493.3203
	1	3.696318000	-0.822862000	0.564851000			1500.8116	1506.0661	1583.8740
	1	1.786023000	-1.929433000	-0.566094000			2971.7075	2988.5078	3027.1498
	1	2.590429000	0.111765000	1.556452000			3028.8751	3032.2677	3037.1539
	1	1.046721000	1.886485000	0.400539000			3041.2150	3041.4560	3045.8947
	1	1.177489000	2.102325000	-1.336503000			3080.1807	3080.7133	3085.5863
	1	2.844428000	0.278658000	-1.476944000			3087.3700	3096.5546	3097.5873
	1	3.386427000	1.492689000	-0.331806000			3099.3110	3102.9053	3781.3414
	8	-1.613539000	2.082869000	1.557206000					
	1	-1.556292000	1.242446000	2.039352000					
TS2e (C_1)	6	-1.480998000	0.345975000	0.356624000	-467.6138065	0.272491	-460.1906	48.2149	62.7550
	6	-0.054767000	0.344365000	-0.162463000			125.8771	138.7548	145.7808
	6	0.642115000	-0.972596000	0.219150000			237.6036	303.2692	305.0713
	6	-0.162889000	-2.171738000	-0.274240000			353.6113	358.8097	402.9916
	6	-1.597322000	-2.147909000	0.245376000			411.2109	456.6675	493.6425
	6	-2.295156000	-0.838539000	-0.132478000			530.9769	564.4636	637.3140
	1	-0.093889000	0.384373000	-1.259615000			780.3491	836.2336	843.0898
	1	-1.486939000	0.400633000	1.450573000			860.8683	862.7595	887.3530
	1	-1.988887000	1.306150000	-0.008239000			903.9668	930.8019	956.6883
	1	-0.173875000	-2.158875000	-1.369776000			1001.9404	1007.4197	1010.1351
	1	0.335089000	-3.097051000	0.024202000			1056.0111	1071.1292	1074.9238
	1	-2.160282000	-2.997039000	-0.144438000			1078.4577	1110.6517	1119.6364

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	-1.586678000	-2.246465000	1.335016000			1160.8614	1165.9577	1167.7381
	1	-2.388987000	-0.782436000	-1.220435000			1187.7562	1235.9857	1250.1584
	1	-3.304055000	-0.807302000	0.278986000			1262.7004	1281.7408	1299.0901
	1	0.676910000	-1.013528000	1.317137000			1313.3577	1317.9934	1319.4784
	6	2.077482000	-0.988527000	-0.300185000			1338.1811	1362.0442	1366.8225
	6	0.742762000	1.548341000	0.329895000			1371.7526	1373.2624	1381.9874
	6	2.178880000	1.522795000	-0.185224000			1385.3475	1389.6106	1392.6518
	6	2.873810000	0.216681000	0.191900000			1403.5100	1483.0701	1489.4862
	1	2.565624000	-1.918839000	-0.000820000			1489.6625	1491.4511	1493.9009
	1	3.886105000	0.193379000	-0.213852000			1502.0963	1506.2764	1686.7897
	1	2.052287000	-0.983754000	-1.395628000			2991.2550	3005.1723	3026.9333
	1	2.967703000	0.162506000	1.281025000			3030.2552	3035.5394	3040.2602
	1	0.751271000	1.537761000	1.426176000			3044.4311	3046.7659	3047.6043
	1	0.239037000	2.466520000	0.020467000			3057.7325	3080.8714	3086.0219
	1	2.168018000	1.621073000	-1.275008000			3088.9440	3096.2109	3098.6568
	1	2.736311000	2.376222000	0.203026000			3099.5285	3109.3192	3783.8678
	8	-2.545822000	2.667676000	-0.338702000					
	1	-2.371689000	3.062187000	0.530697000					
TS3a (C_1)	6	-0.958902000	-1.088471000	-1.026374000	-467.6139986	0.272210	-509.4359	41.4401	44.4653
	6	0.218036000	-0.652038000	-0.157883000			113.8702	126.4743	140.3928
	6	0.442761000	0.860948000	-0.265191000			226.8365	299.3120	309.5023
	6	-0.830385000	1.623402000	0.093334000			343.6318	349.1427	405.4408
	6	-2.011315000	1.196679000	-0.773472000			413.6758	461.1078	495.0191
	6	-2.219147000	-0.306576000	-0.699306000			520.8052	555.3516	689.4058
	1	-0.041058000	-0.868860000	0.887315000			765.9140	815.7820	844.5522
	1	-0.703539000	-0.921796000	-2.080763000			859.0309	863.5592	879.8460
	1	-1.132404000	-2.160174000	-0.908070000			907.1656	929.4503	938.4924
	1	-1.072277000	1.427169000	1.143173000			999.6359	1004.8775	1009.5487
	1	-0.658692000	2.697932000	-0.000917000			1057.1906	1068.5614	1078.3364
	1	-2.918704000	1.721529000	-0.472432000			1078.8417	1109.9273	1127.2253
	1	-1.815028000	1.469598000	-1.816832000			1159.6548	1167.4814	1183.7413
	1	-2.471509000	-0.544475000	0.391770000			1184.9273	1234.8397	1248.8660
	1	-3.075951000	-0.635886000	-1.288418000			1267.4633	1286.5417	1298.0068
	1	0.690011000	1.079670000	-1.314476000			1306.9516	1324.7475	1343.5182
	6	1.624340000	1.293649000	0.598724000			1350.8576	1364.6625	1368.5653

Species	Cartesian coordinate (Å)				$E_{elec}^{0\ K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	6	1.491465000	-1.418101000	-0.505451000			1377.2318	1383.8318	1385.5208
	6	2.669171000	-0.980555000	0.360310000			1389.3938	1392.4994	1410.0101
	6	2.895642000	0.524999000	0.249723000			1413.9095	1472.6396	1481.7305
	1	1.784786000	2.369103000	0.492258000			1484.1358	1487.8731	1491.6583
	1	3.717221000	0.835504000	0.896935000			1495.5204	1504.2995	1651.8827
	1	1.370641000	1.114342000	1.649543000			2996.0573	3009.7924	3019.1156
	1	3.190908000	0.767920000	-0.776041000			3025.9851	3028.7927	3031.3572
	1	1.731382000	-1.237878000	-1.559873000			3037.8453	3041.4702	3044.2683
	1	1.316626000	-2.491461000	-0.400872000			3075.7050	3077.8257	3080.6020
	1	2.458350000	-1.234162000	1.403872000			3084.8209	3086.9746	3089.3994
	1	3.571784000	-1.524373000	0.077756000			3093.9864	3094.5135	3781.1670
	8	-2.777372000	-0.867985000	1.845828000					
	1	-3.653557000	-1.243430000	1.662957000					
TS3e (C_1)	6	-1.008805000	-1.129316000	0.092275000	-467.6129562	0.272280	-651.7650	43.5436	64.6213
	6	0.404206000	-0.611011000	0.373565000			127.8520	142.4893	146.0790
	6	0.610047000	0.771999000	-0.254080000			225.0018	281.5019	299.0216
	6	-0.454693000	1.752230000	0.229118000			344.9863	352.8343	399.2289
	6	-1.866051000	1.234486000	-0.052555000			410.6762	454.5575	495.2533
	6	-2.058787000	-0.140526000	0.562403000			513.8340	562.5881	678.9324
	1	0.515961000	-0.493082000	1.460890000			770.5687	816.7227	839.9581
	1	-1.118928000	-1.283279000	-0.986581000			856.8827	870.1973	879.2206
	1	-1.152918000	-2.100937000	0.568035000			903.5302	926.2980	943.2443
	1	-0.331667000	1.901085000	1.307649000			997.5422	1006.0253	1014.4253
	1	-0.307024000	2.726375000	-0.242380000			1048.0679	1066.0038	1074.5862
	1	-2.611582000	1.934946000	0.327975000			1083.5231	1114.9692	1122.2885
	1	-2.006908000	1.163573000	-1.136208000			1155.6299	1163.2502	1180.2402
	1	-2.087702000	-0.079662000	1.653852000			1185.0554	1238.7454	1251.8321
	1	-3.090388000	-0.550232000	0.267080000			1270.7136	1284.0294	1300.4034
	1	0.494613000	0.653748000	-1.341173000			1307.2668	1321.8678	1339.1301
	6	2.021785000	1.285600000	0.018673000			1344.9089	1358.4057	1367.9524
	6	1.469290000	-1.592713000	-0.107289000			1372.8237	1376.7827	1380.8227
	6	2.879149000	-1.074559000	0.163698000			1387.1432	1388.0234	1397.7490
	6	3.084862000	0.302360000	-0.461964000			1404.7643	1484.7325	1489.2095
	1	2.158677000	2.260658000	-0.454464000			1490.5930	1494.3151	1497.9641
	1	4.082325000	0.679497000	-0.231631000			1501.9255	1507.9413	1648.1053

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	2.134666000	1.441027000	1.097855000			2996.8012	3007.4254	3027.5048
	1	3.023453000	0.212892000	-1.551124000			3029.7430	3032.4501	3036.7774
	1	1.340054000	-1.746389000	-1.184697000			3037.7370	3039.3151	3042.8594
	1	1.318301000	-2.564146000	0.368615000			3063.1451	3084.3610	3086.3499
	1	3.032698000	-1.003022000	1.245058000			3089.1870	3090.2728	3094.9316
	1	3.620629000	-1.779587000	-0.214841000			3099.2322	3100.1226	3789.3864
	8	-4.380107000	-0.785229000	-0.443229000					
	1	-4.459427000	0.117064000	-0.791132000					
PC1 (C_1)	6	1.275343000	0.750680000	-1.282542000	-467.6572124	0.274557	20.0133	32.7480	84.4055
	6	-0.005965000	0.278889000	-0.670829000			89.2047	96.8675	131.4018
	6	-0.014560000	-1.072254000	-0.016073000			202.4759	212.7352	288.5307
	6	1.249627000	-1.318949000	0.810239000			301.3898	322.0237	342.5023
	6	2.519949000	-0.987927000	0.035887000			373.3802	411.9710	414.1839
	6	2.501166000	0.468874000	-0.414212000			464.9875	477.7832	532.1830
	1	0.048605000	1.706650000	1.077433000			567.6867	723.5975	807.0266
	1	1.405883000	0.236402000	-2.249462000			829.2609	850.9795	861.4492
	1	1.204133000	1.815039000	-1.518075000			882.4943	896.2260	928.0292
	1	1.207391000	-0.689432000	1.706110000			929.1099	1001.2905	1003.0187
	1	1.259238000	-2.356063000	1.151494000			1018.9446	1054.4464	1081.8018
	1	3.398606000	-1.184573000	0.651220000			1087.7066	1095.8982	1130.6234
	1	2.592164000	-1.639693000	-0.840874000			1132.7961	1165.5282	1173.8759
	1	2.472604000	1.116100000	0.466641000			1182.4614	1200.1029	1246.7245
	1	3.409296000	0.715321000	-0.965008000			1270.9021	1284.7720	1297.7952
	1	-0.024409000	-1.819535000	-0.831348000			1302.2171	1321.8156	1358.6265
	6	-1.276379000	-1.298032000	0.819634000			1364.5866	1365.3222	1371.8082
	6	-1.283286000	0.769939000	-1.275377000			1381.9164	1384.3239	1384.8652
	6	-2.506552000	0.511562000	-0.396648000			1399.0851	1401.0500	1461.2396
	6	-2.547720000	-0.943452000	0.057587000			1473.7567	1482.3637	1490.0005
	1	-1.301773000	-2.335074000	1.160125000			1492.3231	1492.7025	1504.0566
	1	-3.424402000	-1.123378000	0.680916000			1506.6035	1617.9396	2912.0626
	1	-1.214290000	-0.672395000	1.717527000			2947.9462	2951.6809	3025.2268
	1	-2.640159000	-1.594674000	-0.817546000			3031.2435	3038.6203	3039.4579
	1	-1.430765000	0.254310000	-2.239073000			3049.9449	3054.2466	3074.6621
	1	-1.196301000	1.832065000	-1.515088000			3078.7519	3085.9351	3090.2072
	1	-2.459312000	1.161479000	0.481957000			3098.5970	3099.3498	3103.2268

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	-3.415360000	0.773312000	-0.939208000			3104.9258	3744.4645	3925.9284
	8	0.101499000	2.367684000	1.780066000					
	1	-0.172877000	1.906690000	2.575743000					
PC2	6	-1.180986000	0.681270000	-1.172701000	-467.6535205	0.274448	46.7416	71.0088	104.7548
(C_1)	6	0.164330000	0.107715000	-0.880281000			124.2598	139.2380	204.8374
	6	0.159685000	-0.694500000	0.432746000			217.5162	267.8403	288.1095
	6	-0.987669000	-1.699244000	0.441496000			302.1960	337.3507	344.1588
	6	-2.336082000	-1.005767000	0.270094000			403.9295	411.3097	413.9128
	6	-2.377804000	-0.197668000	-1.031754000			457.5350	482.3499	517.5731
	1	0.395937000	-0.620107000	-1.681039000			541.4598	649.9049	777.0800
	1	-1.321709000	1.922068000	0.768554000			831.7697	838.1210	859.5105
	1	-1.238661000	1.558369000	-1.808342000			865.0026	897.2604	909.9820
	1	-0.837627000	-2.420919000	-0.370496000			923.8500	992.0269	998.4393
	1	-0.971710000	-2.267005000	1.374279000			1015.1181	1053.8310	1069.9900
	1	-3.148037000	-1.733886000	0.278256000			1075.9423	1093.4683	1112.8598
	1	-2.496934000	-0.330294000	1.114503000			1128.3413	1137.1482	1162.9588
	1	-2.399231000	-0.905363000	-1.875598000			1176.5375	1207.8453	1249.4373
	1	-3.298837000	0.382883000	-1.098694000			1258.8109	1264.5877	1293.4581
	1	-0.008845000	0.019213000	1.249497000			1305.2148	1313.9955	1330.0693
	6	1.520176000	-1.347989000	0.652638000			1355.6630	1362.8970	1370.0502
	6	1.277353000	1.154213000	-0.873102000			1374.0020	1381.9034	1385.7095
	6	2.639641000	0.508651000	-0.635013000			1388.3669	1401.3399	1414.5338
	6	2.642640000	-0.312980000	0.652239000			1466.5194	1482.7691	1487.7061
	1	1.513422000	-1.902775000	1.593437000			1488.4935	1492.5161	1501.1512
	1	3.609476000	-0.800080000	0.787393000			1503.5616	1620.3009	2915.1724
	1	1.695480000	-2.079667000	-0.144639000			2957.1597	3011.4173	3017.4594
	1	2.503516000	0.360080000	1.503731000			3026.8882	3028.8183	3030.5550
	1	1.071240000	1.876003000	-0.075308000			3036.2555	3043.8742	3072.1761
	1	1.273777000	1.706654000	-1.815602000			3073.9430	3077.5189	3084.2197
	1	2.877993000	-0.145738000	-1.479641000			3085.9786	3090.2673	3095.6605
	1	3.418101000	1.272046000	-0.597011000			3164.5565	3769.4604	3941.4546
	8	-1.266371000	2.228905000	1.682410000					
	1	-1.634086000	3.115073000	1.679261000					
PC3	6	-0.929768000	-1.037232000	-1.247859000	-467.6532838	0.274209	22.4205	46.4001	96.8840
(C_1)	6	0.196613000	-0.638931000	-0.287901000			105.2854	127.6734	155.3676

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	6	0.353796000	0.885060000	-0.237084000			216.0647	240.9930	259.5298
	6	-0.957952000	1.549460000	0.172263000			304.1196	334.2672	347.7686
	6	-2.102044000	1.188176000	-0.779411000			350.6635	409.2976	414.6633
	6	-2.191980000	-0.284470000	-0.998338000			455.3200	479.3759	497.7755
	1	-0.082690000	-0.969140000	0.720790000			548.6717	676.3373	764.1266
	1	-0.582711000	-0.827833000	-2.273743000			813.3432	846.4152	863.6829
	1	-1.100792000	-2.114755000	-1.201975000			871.7456	901.2357	921.5040
	1	-1.212892000	1.223488000	1.185196000			939.7882	986.4028	999.8979
	1	-0.831260000	2.633514000	0.205970000			1007.8515	1048.9249	1077.7996
	1	-3.049918000	1.585384000	-0.414184000			1081.3652	1089.4416	1115.0034
	1	-1.915533000	1.681448000	-1.746411000			1135.5951	1142.5111	1166.6240
	1	-2.466711000	-0.885324000	1.208596000			1168.5320	1206.8864	1232.5674
	1	-3.131207000	-0.710244000	-1.328306000			1269.1227	1284.2775	1293.9234
	1	0.612081000	1.223055000	-1.251716000			1310.3251	1318.8468	1341.1757
	6	1.493768000	1.277034000	0.700493000			1350.1637	1363.8406	1373.2868
	6	1.511483000	-1.315120000	-0.666035000			1377.0803	1381.0560	1389.4293
	6	2.642848000	-0.919117000	0.277860000			1397.0186	1404.3801	1405.3341
	6	2.806488000	0.598008000	0.321105000			1463.1019	1471.5897	1485.4685
	1	1.610729000	2.363118000	0.702973000			1488.5729	1492.5859	1499.1540
	1	3.593435000	0.876324000	1.023432000			1506.0785	1616.9393	2947.0574
	1	1.217434000	0.986721000	1.720078000			2961.0203	2983.4292	3018.5374
	1	3.122156000	0.951981000	-0.665425000			3030.5979	3033.6450	3039.8008
	1	1.775819000	-1.022216000	-1.688738000			3046.8231	3048.1846	3078.2251
	1	1.379680000	-2.399640000	-0.673528000			3082.8788	3084.0062	3090.6803
	1	2.414061000	-1.283642000	1.283765000			3093.9364	3095.2025	3098.5172
	1	3.575836000	-1.394853000	-0.027629000			3178.8725	3767.7480	3931.9035
	8	-2.344213000	-1.026543000	2.155739000					
	1	-3.113316000	-1.522262000	2.444390000					
P1 (C_1)	6	0.187992000	1.471471000	1.277491000	-391.2187471	0.250911	82.6462	114.5425	197.7233
	6	-0.004098000	0.720262000	0.000000000			280.5754	294.6320	318.3949
	6	0.306328000	-0.748372000	0.000000000			340.0870	409.5135	410.8193
	6	-0.208037000	-1.443471000	1.261718000			461.2100	473.3980	527.3799
	6	0.187992000	-0.702310000	2.532769000			563.1777	722.2125	804.7908
	6	-0.343501000	0.726374000	2.500433000			825.1047	845.7064	861.0187
	1	1.267691000	1.648532000	1.423015000			877.9871	896.1535	925.9630

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	1	-0.266211000	2.461994000	1.198268000			926.5110	1000.2764	1003.3798
	1	-1.300586000	-1.494346000	1.205557000			1018.3773	1054.1417	1080.0823
	1	0.157648000	-2.472384000	1.281577000			1085.2615	1093.3850	1128.9024
	1	-0.187688000	-1.229074000	3.411134000			1130.8120	1164.4367	1174.4355
	1	1.279568000	-0.680866000	2.617891000			1182.3039	1201.0044	1247.1380
	1	-1.435879000	0.698114000	2.455735000			1268.9821	1282.3255	1295.9681
	1	-0.072432000	1.261679000	3.411298000			1302.8709	1318.9270	1358.4713
	1	1.409072000	-0.843406000	0.000000000			1362.1306	1363.6550	1368.7279
	6	-0.208037000	-1.443471000	-1.261718000			1377.5623	1381.1491	1382.1301
	6	0.187992000	1.471471000	-1.277491000			1396.8551	1403.7533	1465.0773
	6	-0.343501000	0.726374000	-2.500433000			1476.8597	1480.6956	1487.2312
	6	0.187992000	-0.702310000	-2.532769000			1488.1623	1488.5675	1499.7859
	1	0.157648000	-2.472384000	-1.281577000			1502.8416	2908.7381	2940.4172
	1	-0.187688000	-1.229074000	-3.411134000			2944.4354	3027.8509	3030.1036
	1	-1.300586000	-1.494346000	-1.205557000			3032.0601	3035.1713	3041.9419
	1	1.279568000	-0.680866000	-2.617891000			3042.4850	3068.5844	3072.7731
	1	1.267691000	1.648532000	-1.423015000			3077.0657	3081.8216	3085.4574
	1	-0.266211000	2.461994000	-1.198268000			3086.2172	3092.7398	3093.1089
	1	-1.435879000	0.698114000	-2.455735000					
	1	-0.072432000	1.261679000	-3.411298000					
P2 (C_1)	6	1.252771000	1.451993000	-0.104821000	-391.2156705	0.250099	125.2682	130.4613	205.4528
	6	-0.002491000	0.743910000	0.267229000			278.9405	293.7254	304.5781
	6	0.022692000	-0.708894000	-0.244583000			349.1032	391.2509	405.6767
	6	1.304761000	-1.407057000	0.196578000			419.7500	468.5793	509.4150
	6	2.546737000	-0.671827000	-0.298961000			536.6215	614.0072	773.6658
	6	2.553356000	0.785977000	0.180549000			833.6193	836.6408	857.8383
	1	-0.049444000	0.671847000	1.370146000			865.1231	895.5616	904.0138
	1	1.218258000	2.507076000	-0.344017000			924.5066	989.8902	1000.5811
	1	1.320725000	-1.456926000	1.291698000			1015.7822	1055.2574	1064.7351
	1	1.305750000	-2.438025000	-0.164942000			1070.5607	1099.1430	1114.1339
	1	3.452301000	-1.179558000	0.036213000			1128.2934	1135.7105	1165.5060
	1	2.554558000	-0.684981000	-1.392107000			1175.0259	1204.0723	1246.6100
	1	2.734609000	0.783142000	1.267015000			1256.2728	1261.9014	1290.1269
	1	3.381953000	1.334163000	-0.268052000			1303.0158	1312.5315	1325.7715
	1	0.023767000	-0.659481000	-1.342097000			1349.9244	1354.5477	1364.6878

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	6	-1.234848000	-1.450584000	0.195916000			1367.7158	1376.8294	1381.7108
	6	-1.263595000	1.463594000	-0.202926000			1387.1158	1392.7877	1419.3099
	6	-2.523778000	0.715658000	0.222186000			1474.1278	1481.4981	1486.4833
	6	-2.499638000	-0.731501000	-0.266029000			1488.2449	1491.7290	1497.1555
	1	-1.214432000	-2.472527000	-0.189742000			1503.8211	2919.6691	2956.8403
	1	-3.387654000	-1.262728000	0.079762000			2999.0487	3019.2039	3025.2079
	1	-1.236130000	-1.526011000	1.289292000			3029.1112	3031.4641	3035.4378
	1	-2.532327000	-0.739017000	-1.360064000			3039.8280	3070.5450	3075.9661
	1	-1.231619000	1.542385000	-1.294915000			3076.4801	3084.7102	3088.8425
	1	-1.272942000	2.483569000	0.187678000			3089.4899	3093.0210	3189.4298
	1	-2.590711000	0.723078000	1.314778000					
	1	-3.412466000	1.226387000	-0.151482000					
P3 (C_{2v})	6	-1.271217000	1.504100000	0.133234000	-391.2158883	0.250131	121.3072	140.7159	210.2810
	6	-0.015843000	0.731760000	-0.289679000			251.7929	297.9590	331.2909
	6	-0.056708000	-0.704008000	0.246757000			347.5032	396.0820	412.4704
	6	-1.318709000	-1.423591000	-0.220082000			429.2759	465.5278	494.5783
	6	-2.589348000	-0.679345000	0.202773000			544.4305	642.3723	760.4168
	6	-2.520554000	0.758382000	-0.179148000			810.5863	844.6865	863.2872
	1	-0.013398000	0.666018000	-1.386029000			868.9785	901.8412	919.6736
	1	-1.200602000	1.674348000	1.220977000			936.9721	979.6038	999.3849
	1	-1.276926000	2.492832000	-0.329278000			1006.4878	1046.8598	1068.5370
	1	-1.293053000	-1.499324000	-1.311851000			1079.7634	1083.1422	1114.0207
	1	-1.330938000	-2.443242000	0.171707000			1127.6211	1141.1521	1162.8666
	1	-3.473935000	-1.154668000	-0.221641000			1166.9601	1200.8069	1229.3968
	1	-2.685453000	-0.767433000	1.296670000			1266.0919	1278.1679	1290.7845
	1	-3.423653000	1.296211000	-0.429855000			1299.5847	1314.7559	1332.7477
	1	-0.083870000	-0.640134000	1.344679000			1341.5118	1358.5820	1368.6481
	6	1.204258000	-1.467010000	-0.152690000			1371.2412	1376.8016	1384.7905
	6	1.258101000	1.447202000	0.149984000			1393.1667	1397.1844	1403.9484
	6	2.511069000	0.677665000	-0.256795000			1466.7062	1475.6396	1482.8836
	6	2.473754000	-0.746842000	0.290903000			1487.7337	1490.2797	1493.9185
	1	1.170203000	-2.476284000	0.264099000			1504.8588	2945.2108	2965.2842
	1	3.357025000	-1.301875000	-0.028567000			2987.4939	3005.9366	3024.0771
	1	1.213710000	-1.577342000	-1.243101000			3024.7343	3031.8244	3033.8447
	1	2.501070000	-0.709556000	1.384544000			3037.9836	3067.8004	3071.4090

Species	Cartesian coordinate (Å)				$E_{elec}^{0\ K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	1.239690000	1.556402000	1.240434000			3072.6276	3078.3996	3085.9202
	1	1.275685000	2.457444000	-0.265853000			3086.9311	3092.1392	3204.7124
	1	2.570173000	0.639661000	-1.349061000					
	1	3.405452000	1.197065000	0.090584000					

Frequencies in the parentheses ("( )") are taken from experimental studies.

Table S2: Calculated global rate constants, k_{tot}, of the *trans*-decalin + OH → products over the range of temperature 200 – 2000 K at different pressures, including the HIR treatments, Eckart quantum tunneling effects. Units are in cm^3/molecule/s.

T (K)	0.76 Torr	7.6 Torr	76 Torr	760 Torr	7600 Torr	76000 Torr
200	5.63E-11	5.62E-11	5.63E-11	5.65E-11	5.70E-11	6.46E-11
250	2.93E-11	2.92E-11	2.94E-11	2.94E-11	2.95E-11	3.19E-11
300	**1.94E-11**	**1.94E-11**	**1.93E-11**	**1.93E-11**	**1.96E-11**	**2.03E-11**
400	1.51E-11	1.51E-11	1.51E-11	1.52E-11	1.50E-11	1.54E-11
500	1.81E-11	1.79E-11	1.79E-11	1.79E-11	1.79E-11	1.79E-11
600	2.30E-11	2.30E-11	2.32E-11	2.31E-11	2.30E-11	2.33E-11
700	2.99E-11	3.03E-11	3.01E-11	2.99E-11	3.02E-11	3.00E-11
800	3.83E-11	3.82E-11	3.82E-11	3.81E-11	3.78E-11	3.81E-11
900	4.76E-11	4.75E-11	4.79E-11	4.80E-11	4.79E-11	4.78E-11
1000	5.83E-11	5.81E-11	5.84E-11	5.85E-11	5.83E-11	5.80E-11
1100	7.02E-11	7.05E-11	7.07E-11	7.05E-11	7.01E-11	7.03E-11
1200	8.38E-11	8.40E-11	8.41E-11	8.37E-11	8.39E-11	8.38E-11
1300	9.85E-11	9.89E-11	9.88E-11	9.89E-11	9.88E-11	9.92E-11
1400	1.16E-10	1.15E-10	1.15E-10	1.15E-10	1.15E-10	1.16E-10
1500	1.33E-10	1.32E-10	1.32E-10	1.33E-10	1.33E-10	1.33E-10
1600	1.51E-10	1.52E-10	1.51E-10	1.52E-10	1.51E-10	1.52E-10
1700	1.72E-10	1.73E-10	1.72E-10	1.73E-10	1.72E-10	1.72E-10
1800	1.95E-10	1.94E-10	1.94E-10	1.94E-10	1.95E-10	1.95E-10
1900	2.18E-10	2.17E-10	2.17E-10	2.18E-10	2.18E-10	2.18E-10
2000	2.42E-10	2.42E-10	2.43E-10	2.43E-10	2.44E-10	2.43E-10

Table S3: The calculated Eckart tunneling factor via tight transition state channels over the wide range of temperature 200 – 2000 K.

T (K)	via TS1	via TS2a	via TS2e	via TS3a	via TS3e
200	1.0	1.8	1.2	1.7	1.6
250	1.0	1.5	1.1	1.4	1.4
300	**1.0**	**1.3**	**1.1**	**1.3**	**1.2**
400	1.0	1.2	1.0	1.2	1.1
500	1.0	1.1	1.0	1.1	1.1
600	1.0	1.1	1.0	1.1	1.1
700	1.0	1.1	1.0	1.1	1.0
800	1.0	1.0	1.0	1.0	1.0
900	1.0	1.0	1.0	1.0	1.0
1000	1.0	1.0	1.0	1.0	1.0
1100	1.0	1.0	1.0	1.0	1.0
1200	1.0	1.0	1.0	1.0	1.0
1300	1.0	1.0	1.0	1.0	1.0
1400	1.0	1.0	1.0	1.0	1.0
1500	1.0	1.0	1.0	1.0	1.0
1600	1.0	1.0	1.0	1.0	1.0
1700	1.0	1.0	1.0	1.0	1.0
1800	1.0	1.0	1.0	1.0	1.0
1900	1.0	1.0	1.0	1.0	1.0
2000	1.0	1.0	1.0	1.0	1.0

Table S4: Calculated overall rate constants, k_{tot}, of the *trans*-decalin + OH → products over the range of temperature 200 – 2000 K at P = 760 Torr with and without HIR treatments based on M06-2X/aug-cc-pVTZ level of theory. Units are in cm^3/molecule/s.

T (K)	***trans*-decalin + OH → products (k_tot)**		**HIR factor**
	With HIR	**Without HIR**	
200	5.65E-11	2.48E-11	2.3
250	2.94E-11	1.37E-11	2.1
300	**1.93E-11**	**9.49E-12**	**2.0**
400	1.52E-11	7.22E-12	2.1
500	1.79E-11	8.47E-12	2.1
600	2.31E-11	1.14E-11	2.0
700	2.99E-11	1.53E-11	2.0
800	3.81E-11	2.03E-11	1.9
900	4.80E-11	2.59E-11	1.8
1000	5.85E-11	3.31E-11	1.8
1100	7.05E-11	4.15E-11	1.7
1200	8.37E-11	5.09E-11	1.6
1300	9.89E-11	6.22E-11	1.6
1400	1.15E-10	7.39E-11	1.6
1500	1.33E-10	8.82E-11	1.5
1600	1.52E-10	1.03E-10	1.5
1700	1.73E-10	1.21E-10	1.4
1800	1.94E-10	1.39E-10	1.4
1900	2.18E-10	1.58E-10	1.4
2000	2.43E-10	1.80E-10	1.3

Table S5: Modified Arrhenius format of total temperature-and pressure-dependent rate constants, $k_{tot}(T, P)$, (in cm^3/molecule/s) for the reaction of *trans*-decalin + OH → products at T = 200 – 2000 K & P = 0.76 – 76000 Torr.

No.	Pressure (Torr)	$k_{tot}(T, P) = A \times T^n \times \exp(-E_a/RT)$			
		A [a]	n	E_a/R (K)	Error (%)
1	0.76	1.67×10^{-21}	3.31	-1.32×10^{3}	1.97
2	7.6	1.68×10^{-21}	3.31	-1.32×10^{3}	2.00
3	76	1.68×10^{-21}	3.31	-1.32×10^{3}	2.01
4	760	1.62×10^{-21}	3.31	-1.32×10^{3}	1.97
5	7600	1.53×10^{-21}	3.32	-1.33×10^{3}	2.01
6	76000	1.02×10^{-21}	3.37	-1.38×10^{3}	2.09

[a] Units of [cm^3 $molecule^{-1}$ s^{-1}].

Table S6: Calculated thermodynamic data of the species involved in NASA format for the title reaction.

oh O 1H 1 G 300.000 2500.000 1500.000 1
-2.69563255E-0012.22268930E-003-1.31935314E-0063.31105426E-010-2.89497127E-014 2
-4.27622944E+0039.14731196E+0001.08544341E+000-4.99059779E-0058.22804718E-008 3
-5.95241136E-0111.61691960E-014-4.90100964E+0031.45363723E+000 4
***trans*-decalin** C 10H 18 G 300.000 2500.000 1500.000 1
-3.65912296E+0028.03677753E-001-6.21474634E-0042.11502342E-007-2.67713716E-011 2
9.99426250E+0042.22130207E+0031.62026282E+0011.91485219E-002-3.57535274E-005 3
2.69688071E-008-7.09230020E-012-4.59078215E+0041.27362599E+002 4
rc C 10H 19O 1 G 300.000 2500.000 1500.000 1
2.12791090E+003-4.42988005E+0003.44929729E-003-1.17924844E-0061.49479558E-010 2
-8.43218070E+005-1.13821947E+0041.13233400E+0015.89881031E-002-1.18182431E-004 3
9.32556073E-008-2.52204963E-011-5.02528179E+0041.66419720E+002 4
ts2a C 10H 19O 1 G 300.000 2500.000 1500.000 1
1.09108523E+002-3.04763030E-0013.27179512E-004-1.41168669E-0072.13823023E-011 2
-6.30745226E+004-3.06440458E+0021.63880475E+0012.84517965E-002-6.40172074E-005 3
5.72153114E-008-1.75184890E-011-5.07412135E+0041.37988864E+002 4
ts2e C 10H 19O 1 G 300.000 2500.000 1500.000 1
-4.83919533E+0021.03787886E+000-7.99264926E-0042.72748453E-007-3.47857807E-011 2
1.45214508E+0052.88970293E+0031.12100144E+0016.17698104E-002-1.34730200E-004 3
1.17160901E-007-3.50440138E-011-5.00884087E+0041.60343429E+002 4
ts3a C 10H 19O 1 G 300.000 2500.000 1500.000 1
-1.51859369E+0033.15976609E+000-2.40254799E-0038.02501125E-007-9.94284329E-011 2
5.41011138E+0058.56296028E+0032.32085855E+001-1.56140252E-0023.25972230E-005 3
-2.85725435E-0088.75371159E-012-5.14499246E+0041.08964842E+002 4
ts3e C 10H 19O 1 G 300.000 2500.000 1500.000 1
-8.48318140E+0021.90587507E+000-1.53841963E-0035.42534247E-007-7.06399324E-011 2
2.59464614E+0054.82587164E+0032.43767413E+001-2.78118388E-0026.91636292E-005 3
-6.69426855E-0082.16159328E-011-5.14963657E+0041.04537573E+002 4
ts1 C 10H 19O 1 G 300.000 2500.000 1500.000 1
-1.65738566E+0033.60194590E+000-2.86045912E-0039.96033713E-007-1.28331385E-010 2
5.65717771E+0059.24866084E+0032.63736591E+001-2.98846464E-0025.31427089E-005 3
-3.88378476E-0081.01486188E-011-5.22047180E+0049.40441258E+001 4
p2 C 10H 17 G 300.000 2500.000 1500.000 1
-4.21618061E+0028.66379909E-001-6.27196145E-0041.97915102E-007-2.29449843E-011 2
1.34987705E+0052.54288298E+0032.00293662E+001-5.33767616E-0037.76836645E-006 3
-3.75217263E-0092.59103270E-013-4.11441564E+0041.03767665E+002 4
h2o O 1H 2 G 300.000 2500.000 1500.000 1
4.96772059E+001-1.00540679E-0017.80662284E-005-2.66184635E-0083.36292935E-012 2
-3.08254335E+004-2.58839707E+0021.73948863E+000-3.81888748E-0046.99701434E-007 3
-5.17522021E-0101.35656397E-013-1.26833643E+0043.26581330E+000 4
p3 C 10H 17 G 300.000 2500.000 1500.000 1
7.86893926E+001-1.07262541E-0016.83791688E-005-1.77389001E-0081.48115426E-012 2
-6.69340835E+004-2.26439038E+0021.98945056E+001-5.53080689E-0031.17540947E-005 3
-1.06309422E-0083.39185843E-012-4.11472063E+0041.04391240E+002 4
p1 C 10H 17 G 300.000 2500.000 1500.000 1
-3.95347630E+0028.44256978E-001-6.45611513E-0042.19138294E-007-2.78192976E-011 2
1.21831658E+0052.38711916E+0031.21888334E+0014.17595848E-002-8.76314278E-005 3
7.44422622E-008-2.19106771E-011-4.03823759E+0041.37936132E+002 4

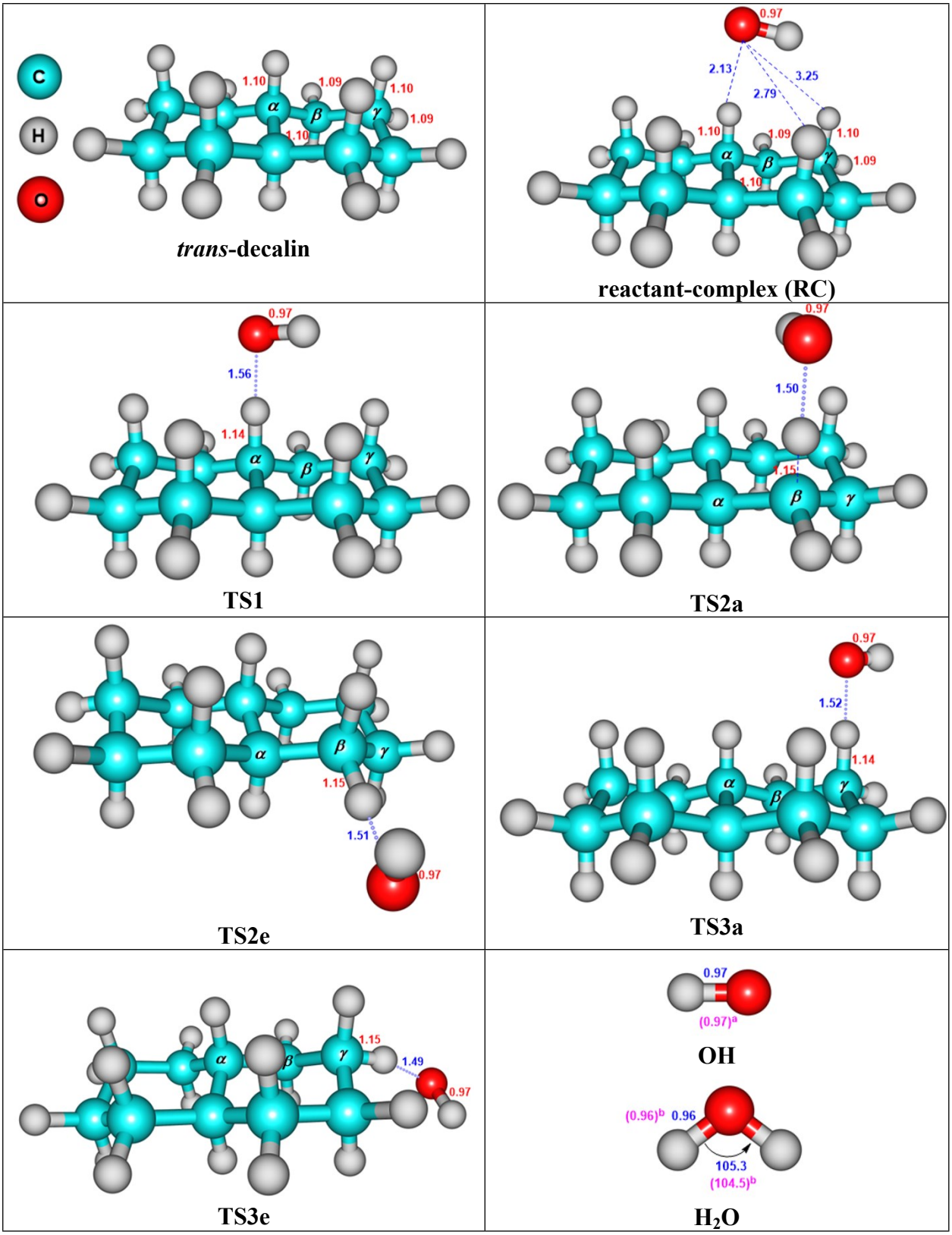
Table S7: High-pressure limit rate constants, $k^{\infty}(T)$, for each of the channel calculated at T = 200 – 2000 K.

T (K)	$k^{\infty}(T)$[a]				
	RC → P1 (via **TS1**)	**RC → P2** (via **TS2a**)	*trans*-decalin + OH → **P2** (via **TS2e**)	**RC → P3** (via **TS3a**)	*trans*-decalin + OH → **P3** (via **TS3e**)
200	1.21E+12	8.45E+10	2.10E-12	6.17E+10	2.39E-12
250	1.19E+12	1.35E+11	2.75E-12	1.29E+11	3.28E-12
300	1.15E+12	1.85E+11	3.47E-12	2.12E+11	4.29E-12
400	1.06E+12	2.69E+11	5.17E-12	3.89E+11	6.67E-12
500	9.90E+11	3.33E+11	7.22E-12	5.53E+11	9.57E-12
600	9.35E+11	3.81E+11	9.69E-12	6.96E+11	1.31E-11
700	8.93E+11	4.19E+11	1.26E-11	8.18E+11	1.72E-11
800	8.60E+11	4.50E+11	1.60E-11	9.22E+11	2.21E-11
900	8.34E+11	4.75E+11	1.99E-11	1.01E+12	2.77E-11
1000	8.13E+11	4.97E+11	2.43E-11	1.09E+12	3.41E-11
1100	7.95E+11	5.14E+11	2.93E-11	1.15E+12	4.12E-11
1200	7.80E+11	5.29E+11	3.48E-11	1.21E+12	4.92E-11
1300	7.67E+11	5.42E+11	4.08E-11	1.26E+12	5.80E-11
1400	7.55E+11	5.53E+11	4.75E-11	1.31E+12	6.76E-11
1500	7.45E+11	5.62E+11	5.46E-11	1.34E+12	7.80E-11
1600	7.35E+11	5.70E+11	6.24E-11	1.38E+12	8.94E-11
1700	7.25E+11	5.76E+11	7.07E-11	1.40E+12	1.02E-10
1800	7.17E+11	5.81E+11	7.96E-11	1.43E+12	1.15E-10
1900	7.09E+11	5.85E+11	8.91E-11	1.45E+12	1.28E-10
2000	7.01E+11	5.89E+11	9.92E-11	1.47E+12	1.43E-10

[a] Units of [1/s] for first-order reactions and [cm^3/molecule/s] for second-order reactions.

Table S8: Relative Gibbs free energy calculated at different temperatures (e.g., 0, 200, 300, 500, 800, 1000, 1200 and 2000 K), obtained at M06-2X/aug-cc-pVTZ.

Species	0 K	200 K	300 K	500 K	800 K	1000 K	1200 K	2000 K
RC	-1.7	2.2	4.2	8.0	13.3	16.7	19.9	32.0
TS1	-1.6	2.7	5.2	10.3	18.0	23.1	28.1	48.2
TS2a	-0.2	4.0	6.5	11.5	19.1	24.1	29.1	49.0
TS2e	0.4	4.4	6.8	11.5	18.6	23.3	28.0	46.5
TS3a	0.1	4.1	6.4	11.0	18.0	22.6	27.2	45.3
TS3e	0.8	4.5	6.7	11.3	18.1	22.7	27.2	45.1
P1 + H_2O	-21.6	-22.7	-23.4	-24.8	-27.0	-28.4	-29.8	-35.0
P2 + H_2O	-20.2	-21.1	-21.8	-23.1	-25.3	-26.7	-28.1	-33.5
P3 + H_2O	-20.3	-21.2	-21.8	-23.2	-25.3	-26.7	-28.0	-33.2


C
H
O
1.10
1.09
1.10
1.09
1.10
α
β
γ
trans-decalin
0.97
2.13
3.25
2.79
1.10
1.09
1.10
1.09
1.10
α
β
γ
reactant-complex (RC)
0.97
1.56
1.14
α
β
γ
TS1
0.97
1.50
1.15
α
β
γ
TS2a
α
β
γ
1.15
1.51
0.97
TS2e
0.97
1.52
1.14
α
β
γ
TS3a
α
β
γ
1.15
1.49
0.97
TS3e
0.97
(0.97)a
OH
(0.96)b
0.96
105.3
(104.5)b
H2O

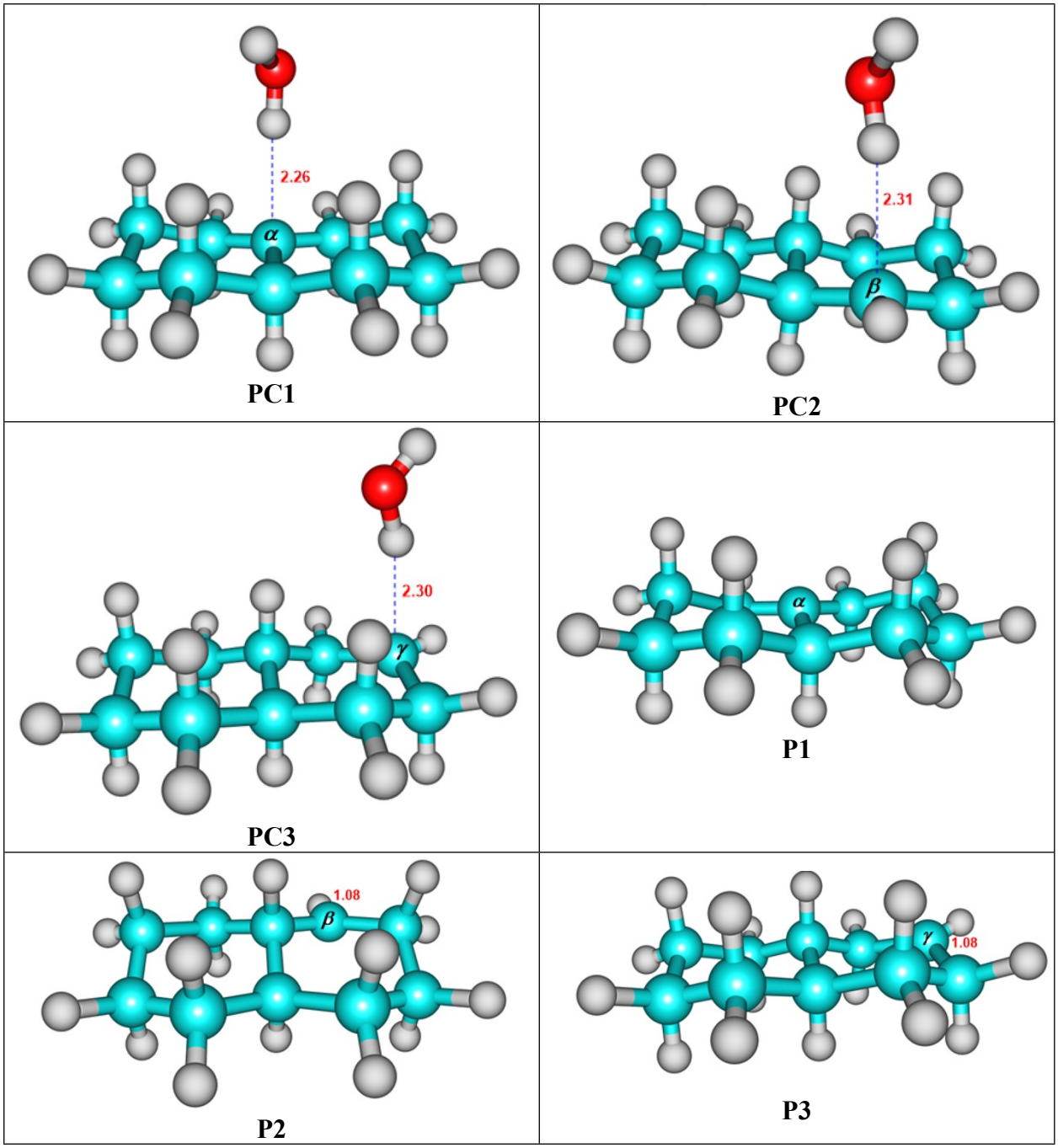


Figure S1: M06-2X/aug-cc-pVTZ optimized geometries for the species involved in the title reaction. All structures were obtained for the lowest-energy conformer of a given species. Bond lengths and bond angles are in Å and degree (°), respectively. [a, b] are taken from the experimental data[5, 7], respectively.

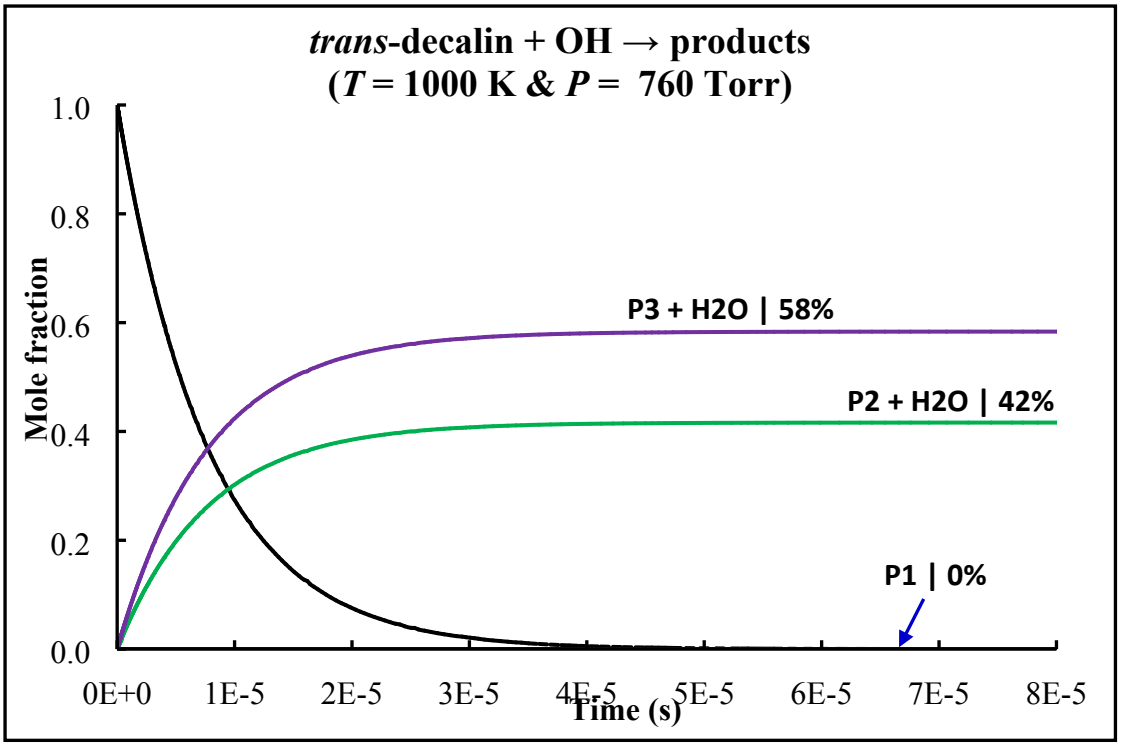


Figure S2: Time-resolved species profiles for the reaction of *trans*-decalin + OH → Products, conducted at $T = 1000$ K and atmospheric pressure, using the stochastic (with 10^6 trials) scheme with $[OH]/[[N_2] = 3.0\times10^{-4}$ and $[trans\text{-decalin}]_0 >> [OH]_0$ (N_2 is the buffer gas).

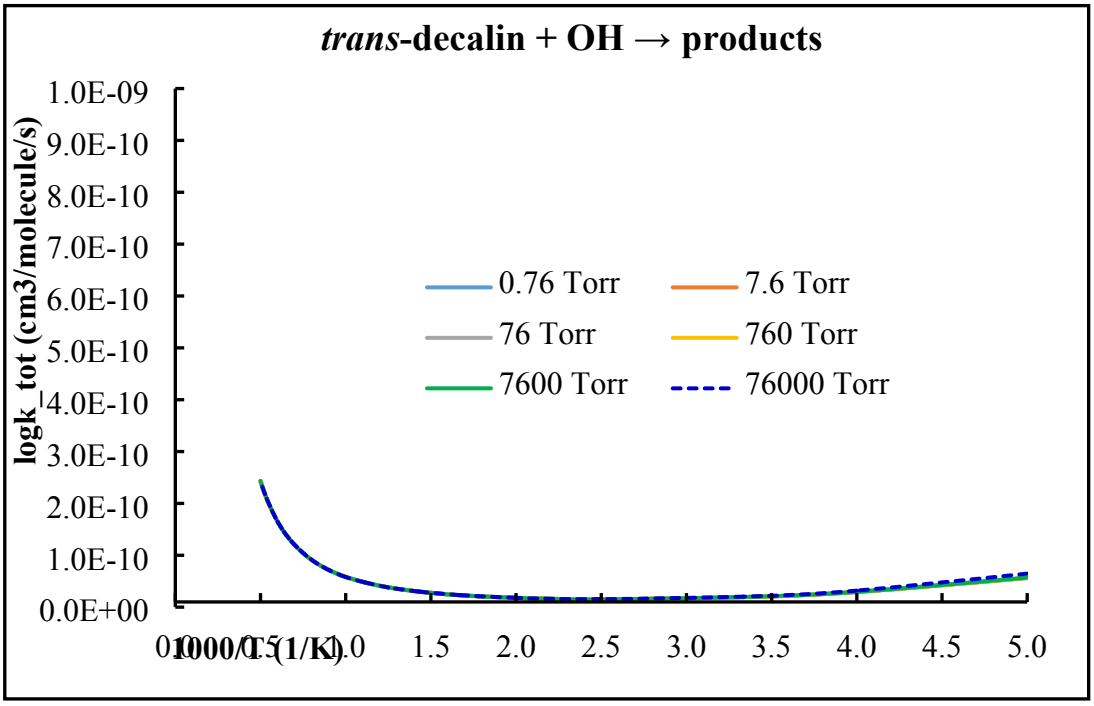
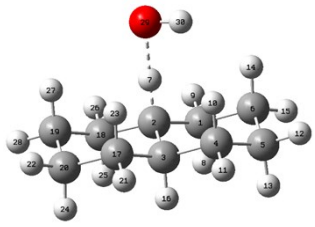
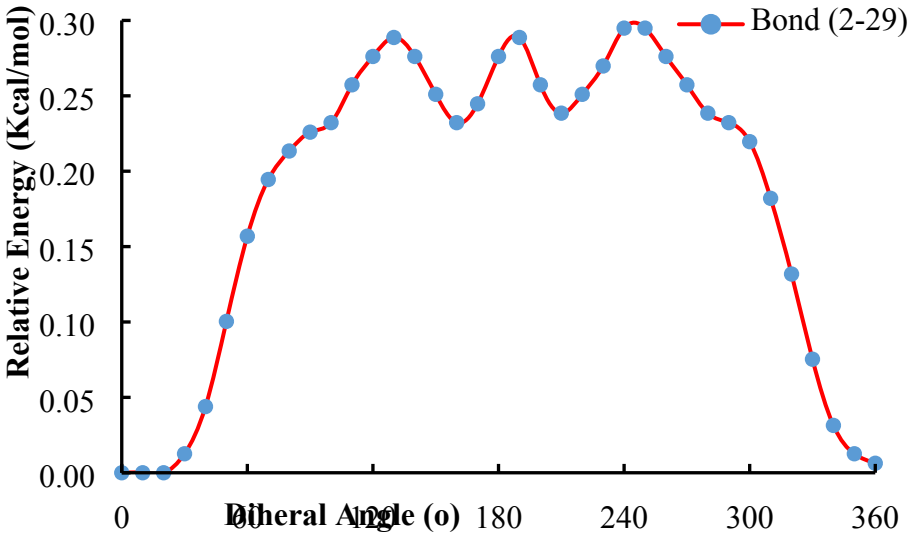
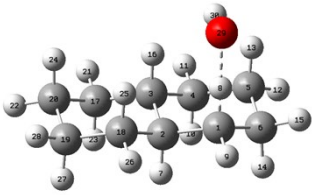
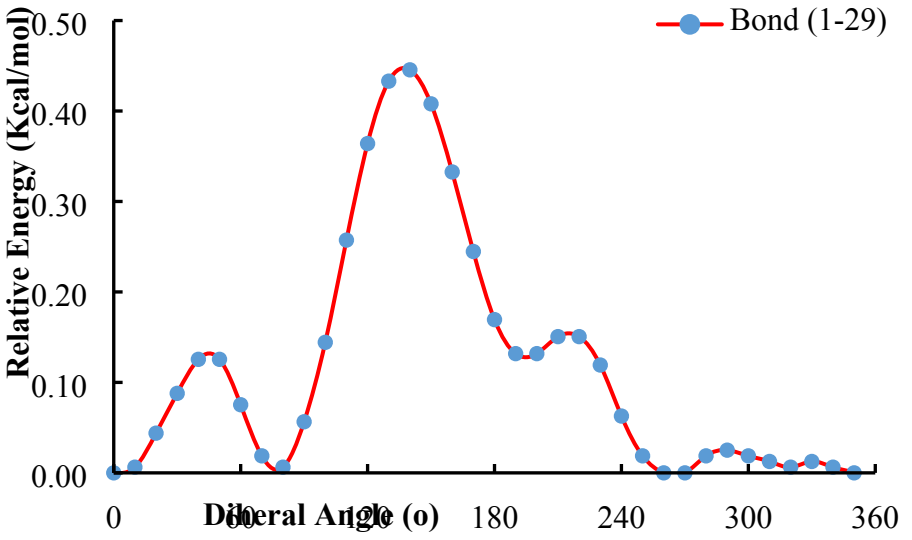
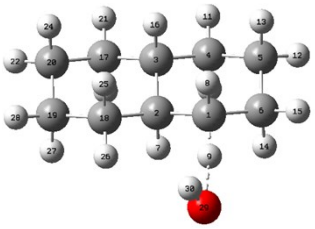
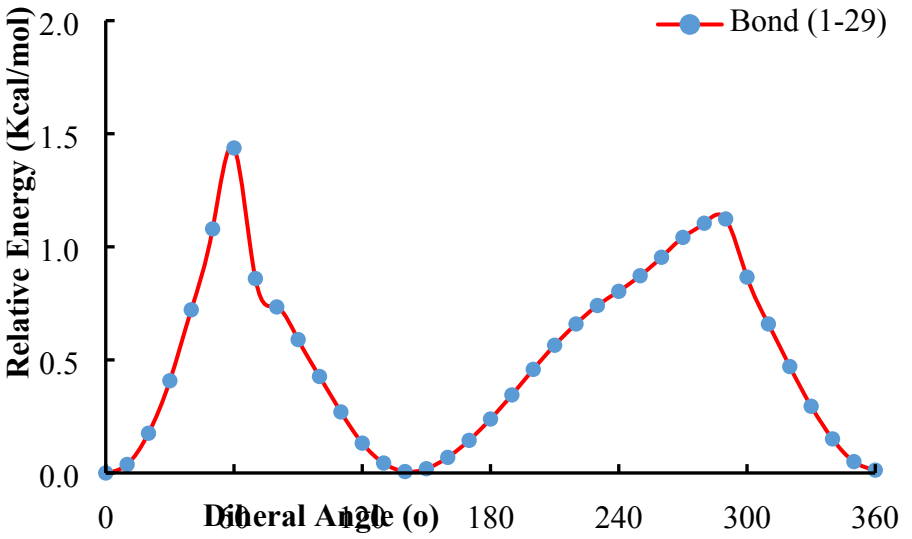


Figure S3: Calculated global rate constant, k_{tot}, as a function of temperature at different pressures (e.g., 0.76, 7.6, 76, 760, 7600 and 76000 Torr).

Species	Potential energy surfaces for the internal rotations
 TS1	
 TS2a	
 TS2e	

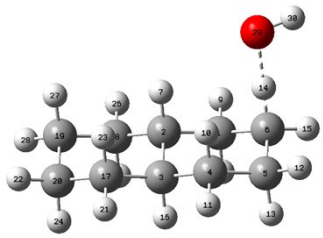
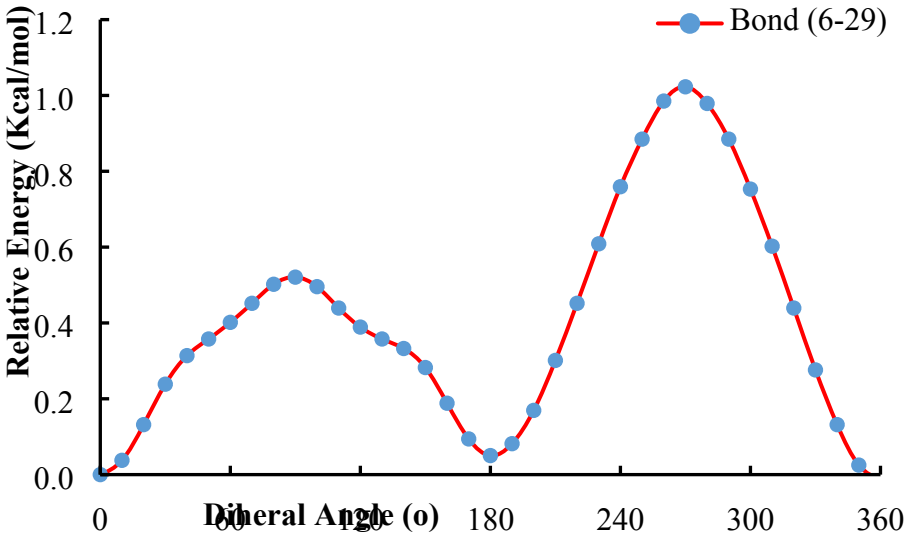
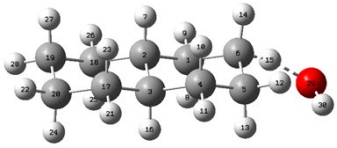
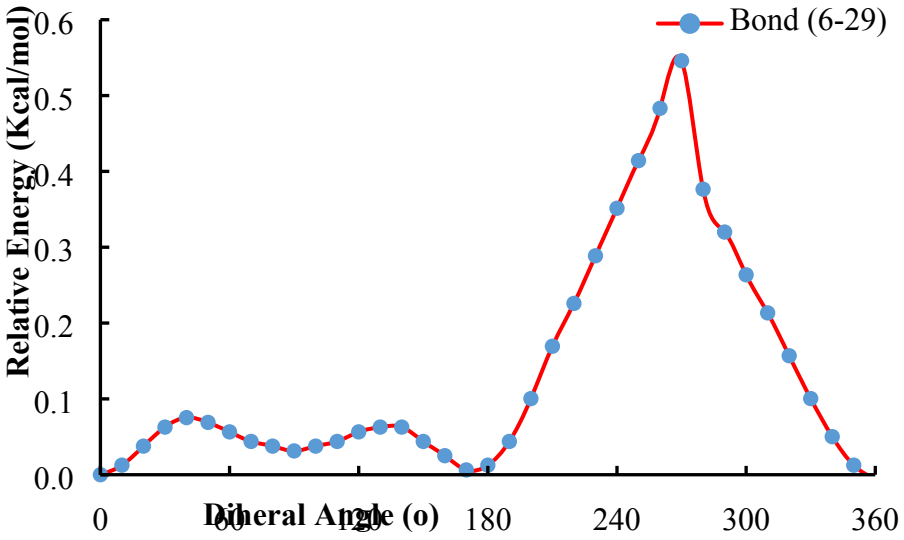
Species	Potential energy surfaces for the internal rotations
 TS3a	
 TS3e	

Figure S4: Hindrance potentials for the species involved in the *trans*-decalin + OH reaction, calculated at M06-2X/cc-pVDZ level of theory.

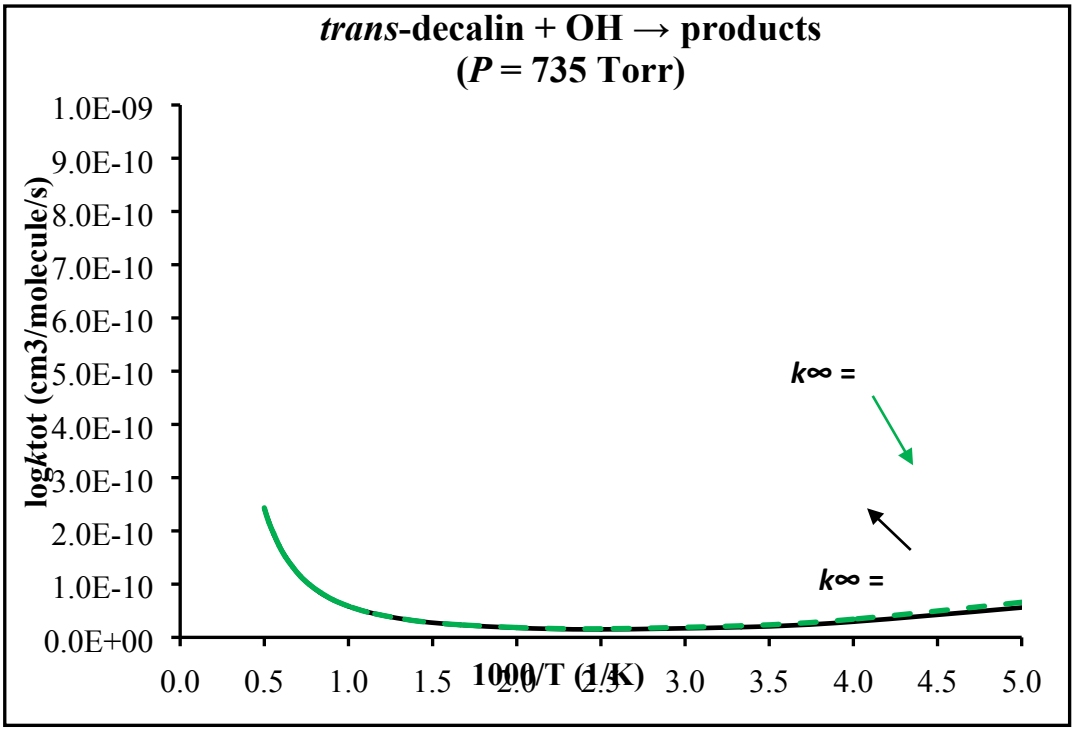


Figure S5: Comparison of the computed global rate constant, k_{tot}, for *trans*-decalin + OH → Products reaction by using the $k^{\infty}(T)$ of 4.0×10^{-10} (solid line) and 8.0×10^{-10} (dashed line) cm^3/molecule/s, at T = 200 – 2000 K & P = 735 Torr.

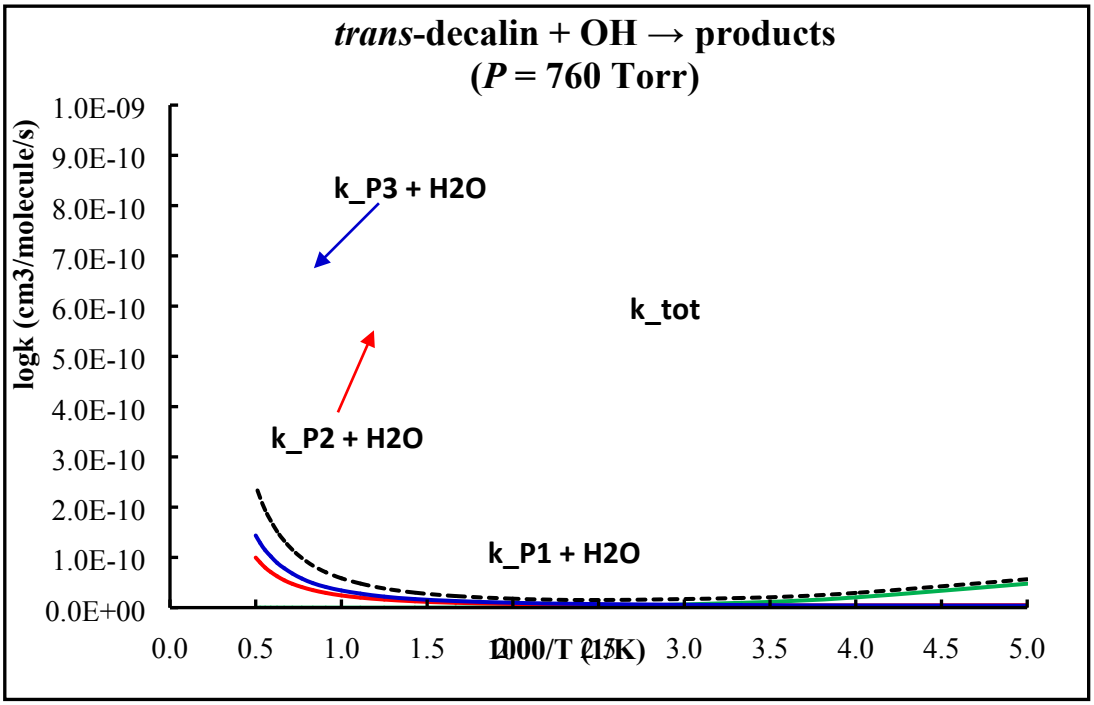


Figure S6: Arrhenius plot of rate constants for the reaction of *trans*-decalin + OH → Products at P = 760 Torr.

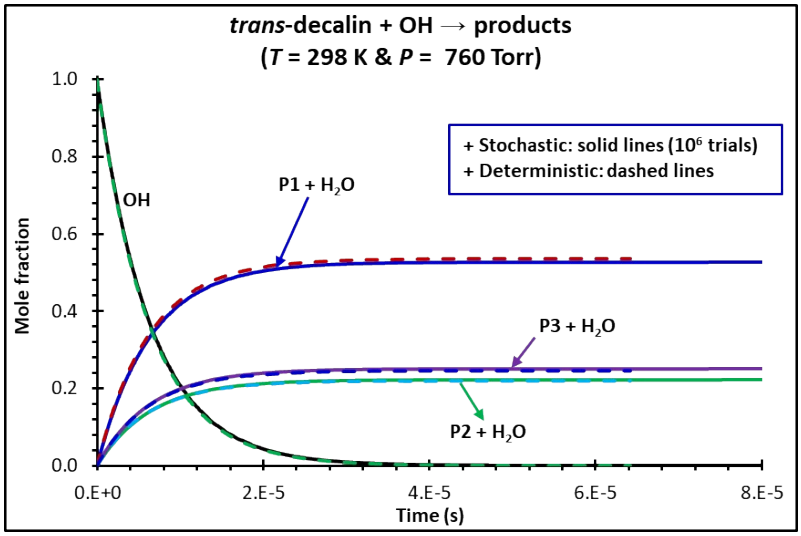


Figure S7: Comparison of time-resolved species profiles for the reaction of *trans*-decalin + OH → Products, studied at the atmospheric condition using the stochastic (solid lines) and deterministic (dashed lines) models with [OH]/[[N_2] = 3.0×10^{-4} and [*trans*-decalin]$_0$ >> [OH]$_0$ (N_2 is the third-body gas).

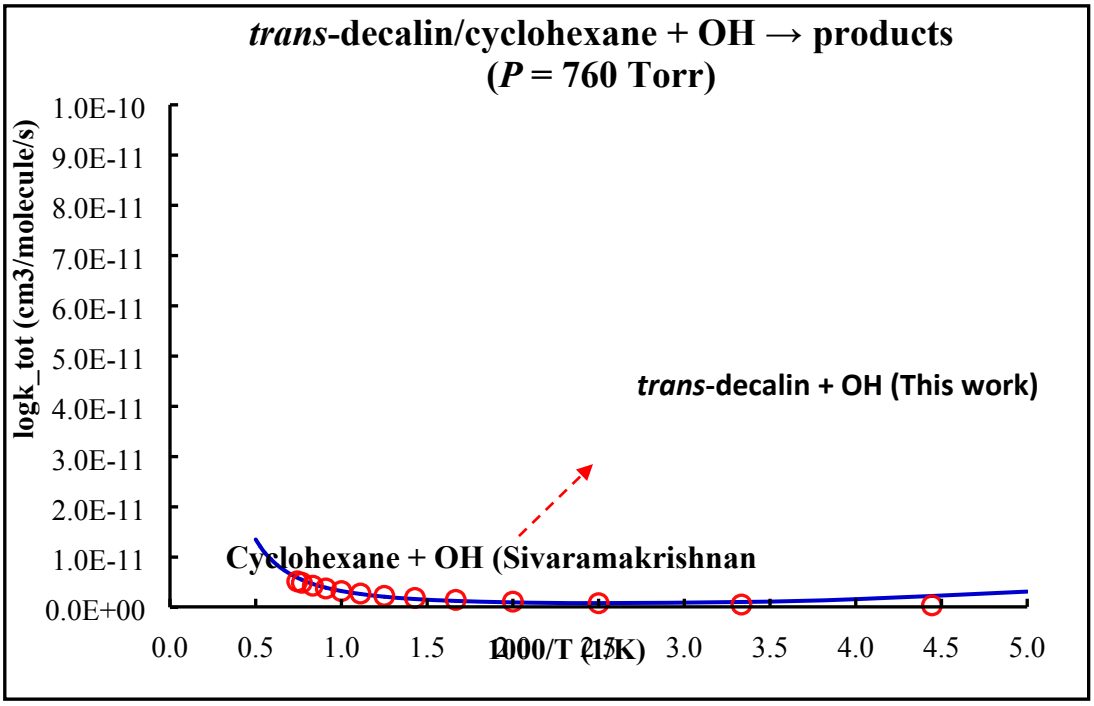


Figure S8: Comparison of the rate constants on a per hydrogen basis between the reactions of trans-decalin + OH (solid line) and cyclohexane + OH[8] (symbol).

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