

Chemical kinetics of H-abstractions from dimethyl amine by H, CH₃, OH and HO₂ radicals with multi-structural torsional anharmonicity

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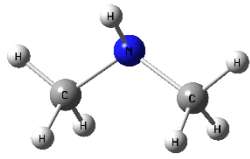
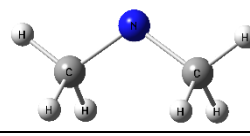
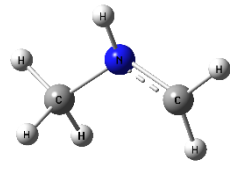
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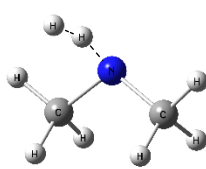
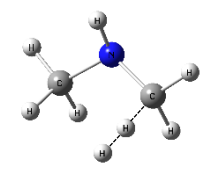
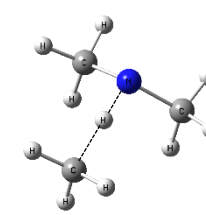
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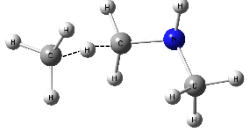
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Table S1: Optimized ground geometries and frequencies for involved species in hydrogen abstraction from DMA by H/CH₃/OH/HO₂ radicals at BHandHLYP/cc-pVTZ level

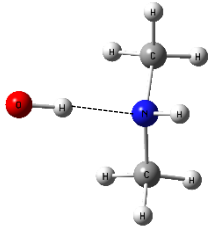
DMA												
Geometry				Frequency (cm ⁻¹)								
N	0.015431	0.571404	0.000000	230.9903	266.4736	393.8462	795.7013	978.8876				
H	-0.777616	1.183765	0.000000	1074.1769	1143.9036	1226.5776	1235.9092	1317.8331				
C	0.026517	-0.221859	1.204650	1496.9604	1525.5063	1532.9725	1542.8525	1550.0842				
H	0.959788	-0.770718	1.268936	1571.1400	1574.5726	3021.6735	3026.0300	3131.1304				
H	-0.033688	0.423213	2.072069	3131.6048	3176.5074	3177.3093	3657.1043					
H	-0.787071	-0.950105	1.261843	Rotational constants (cm ⁻¹)								
C	0.026517	-0.221859	-1.204650	1.1833								
H	-0.033688	0.423213	-2.072069	0.3147								
H	0.959788	-0.770718	-1.268936	0.2781								
H	-0.787071	-0.950105	-1.261843									
CH3NCH3												
Geometry				Frequency (cm ⁻¹)								
N	0.000119	0.624769	-0.000000	87.0163	154.2480	443.0307	959.7387	980.3759				
C	0.000006	-0.173869	1.184366	1056.3653	1065.9719	1259.8961	1265.5126	1453.0755				
H	0.874836	-0.824974	1.217854	1475.3679	1518.6631	1531.0946	1543.9879	1550.0739				
H	0.000388	0.452871	2.065509	3037.6387	3048.1852	3079.4368	3087.2726	3182.5450				
H	-0.875405	-0.824185	1.218108	3183.9211								
C	0.000006	-0.173869	-1.184366	Rotational constants (cm ⁻¹)								
H	0.000388	0.452871	-2.065509	1.3672								
H	0.874836	-0.824974	-1.217854	0.3282								
H	-0.875405	-0.824185	-1.218108	0.2391								
CH3NHCH2												
Geometry				Frequency (cm ⁻¹)								
N	0.088994	0.470569	-0.133454	199.4894	336.1822	398.4162	636.1980	663.3198				
H	0.112217	1.404631	0.219395	999.9298	1078.1535	1184.2811	1297.7729	1341.8932				
C	1.243640	-0.247062	0.075802	1502.9026	1529.4742	1540.2602	1557.3662	1596.0332				
H	1.236402	-1.274403	-0.235388	3066.8493	3146.8675	3187.6905	3220.7647	3332.5736				
H	2.167424	0.296484	0.042585	3709.7885								
C	-1.180407	-0.186996	0.032216	Rotational constants (cm ⁻¹)								
H	-1.978582	0.472413	-0.282154	1.4551								
H	-1.211418	-1.068666	-0.596694	0.3308								
H	-1.369837	-0.500207	1.057862	0.2875								

Reaction 1 DMA + H												
TS1a												
Geometry				Frequency (cm ⁻¹)								
N	-0.084637	0.519201	0.000000	-1812.8433i								
H	0.941366	1.125274	0.000000	195.5896	234.9513	392.1005	407.5188	415.4201				
C	-0.104718	-0.279195	-1.200922	936.0389	1015.1564	1066.0915	1128.3667	1211.6645				
H	-1.087622	-0.731468	-1.295210	1214.0795	1282.2066	1414.8956	1483.4622	1506.0576				
H	0.059116	0.351964	-2.063864	1524.8846	1541.4404	1545.4236	1558.0565	1624.2873				
H	0.630396	-1.082774	-1.205161	3065.5576	3068.7998	3129.1528	3131.4058	3189.0718				
C	-0.104718	-0.279195	1.200922	3189.4737								
H	0.059116	0.351964	2.063864	Rotational constants (cm ⁻¹)								
H	-1.087622	-0.731468	1.295210	0.8267								
H	0.630396	-1.082774	1.205161	0.3051								
H	1.902966	1.311802	0.000000	0.2625								
TS1b												
Geometry				Frequency (cm ⁻¹)								
N	-0.098176	-0.578035	-0.175900	-1345.7554i								
H	-0.088680	-0.913448	-1.118698	188.2461	210.6808	315.7222	423.4028	553.6213				
C	-1.260708	0.230476	0.099932	747.2667	997.2472	1085.8734	1140.5646	1208.5513				
H	-2.153321	-0.293005	-0.215686	1263.2536	1308.6280	1320.1204	1392.8155	1407.8903				
H	-1.335612	0.400438	1.167679	1505.8587	1532.1384	1541.0633	1555.7950	1581.0684				
H	-1.234275	1.202590	-0.392519	3060.4829	3142.1298	3145.0115	3188.6224	3222.5530				
C	1.134565	-0.026350	0.205229	3681.9127								
H	1.973093	-0.658527	-0.048377	Rotational constants (cm ⁻¹)								
H	1.378827	1.066251	-0.399638	0.8589								
H	1.153269	0.261241	1.248264	0.2875								
H	1.552554	1.942538	-0.917206	0.2571								
Reaction 2 DMA + CH ₃												
TS2a												
Geometry				Frequency (cm ⁻¹)								
N	0.422420	-0.000032	-0.519785	-2191.9497i								
H	-0.772144	-0.000027	-0.363793	45.8900	139.7062	165.0583	209.4477	255.7569				
C	0.913649	1.196369	0.116359	406.6016	542.2287	557.6695	570.7919	958.4118				
H	1.979933	1.284445	-0.073495	1075.5876	1132.7774	1149.6305	1199.1240	1232.8238				
H	0.428329	2.065822	-0.307667	1281.2522	1345.3555	1472.0519	1483.4035	1484.3709				
H	0.772113	1.209123	1.198488	1507.1020	1527.8311	1541.8246	1543.7822	1552.7138				
C	0.913656	-1.196359	0.116495	1559.0535	3041.8602	3045.5897	3116.6351	3119.2508				
H	0.428339	-2.065863	-0.307431	3140.2928	3177.9935	3178.8533	3272.3728	3273.4462				
H	1.979940	-1.284451	-0.073350	Rotational constants (cm ⁻¹)								
H	0.772121	-1.208990	1.198625	0.2818								
C	-2.076071	-0.000012	0.076464	0.1533								
H	-2.034965	0.000059	1.153463	0.1110								
H	-2.487409	0.902818	-0.344782									
H	-2.487392	-0.902905	-0.344664									
TS2a												
Geometry				Frequency (cm ⁻¹)								

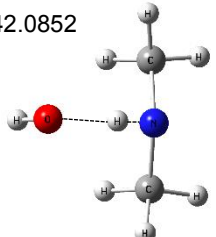
N	-1.109764	0.416071	-0.362621	-1842.0329i				
H	-1.022225	0.397941	-1.359555	30.8608	92.9020	130.3947	239.1774	365.2929
C	-1.485696	-0.873241	0.162677	387.3627	470.2143	575.0604	671.4591	765.3315
H	-1.754440	-0.770907	1.207929	996.9640	1092.1860	1151.5022	1171.9508	1220.4996
H	-2.353968	-1.244805	-0.365790	1254.7484	1328.9868	1456.4612	1460.0176	1496.8955
H	-0.694247	-1.620470	0.094937	1502.0086	1506.1617	1533.0826	1541.4685	1554.0046
C	0.006079	1.024598	0.252506	1577.7873	3053.3351	3131.8144	3137.4399	3139.2797
H	0.241225	1.984256	-0.186475	3182.9551	3208.3696	3266.7403	3270.5214	3675.8118
H	-0.121141	1.108699	1.324539	Rotational constants (cm ⁻¹)				
H	1.090769	0.335805	0.119109	0.3464				
C	2.298212	-0.420096	-0.072088	0.1136				
H	2.222273	-0.802786	-1.077255	0.0952				
H	3.089472	0.300170	0.058124					
H	2.280425	-1.185577	0.686314					

Reaction 3 DMA + OH

RC3

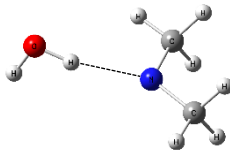
Geometry				Frequency (cm ⁻¹)				
N	-0.378743	-0.007959	0.420287	51.3256	76.3222	193.6686	224.3438	284.9885
H	-0.504723	-0.012255	1.415526	402.7662	630.8289	782.7158	885.5817	972.1496
C	-0.898588	-1.238845	-0.141343	1076.2168	1141.3743	1216.0452	1252.9017	1318.3611
H	-0.648139	-1.287185	-1.194266	1501.9018	1528.6239	1532.8821	1552.5950	1554.6140
H	-0.438470	-2.087216	0.347312	1571.1814	1573.1200	3060.2227	3062.9811	3150.5924
H	-1.981086	-1.327900	-0.049609	3152.9222	3192.5012	3192.7237	3497.1900	3646.0912
C	-0.989955	1.179715	-0.142372	Rotational constants (cm ⁻¹)				
H	-0.595044	2.060807	0.345430	0.2875				
H	-0.744064	1.245799	-1.195417	0.1220				
H	-2.076077	1.186999	-0.050533	0.0936				
O	2.427632	0.094783	-0.147468					
H	1.474283	0.060568	0.075825					

TS3a

Geometry				Frequency (cm ⁻¹)				
N	0.360977	-0.000194	-0.465463	-1045.3728i				
H	-0.700157	-0.031686	-0.614286	39.2265	142.4711	169.5375	199.4986	232.8129
C	0.790946	1.216551	0.166031	382.7887	569.4029	767.8899	979.3696	1078.3969
H	1.855857	1.347046	-0.002394	1136.9325	1191.2751	1223.9888	1300.9594	1479.6731
H	0.269145	2.056720	-0.268390	1496.9689	1506.3793	1526.0181	1541.6423	1545.4276
H	0.629188	1.222127	1.244492	1559.8873	1936.9450	3051.9358	3053.7720	3124.3546
C	0.866917	-1.202712	0.136283	3126.9322	3205.9555	3206.5954	3942.0852	
H	0.398533	-2.063045	-0.319056	Rotational constants (cm ⁻¹)				
H	1.937787	-1.261972	-0.034468	0.2901				
H	0.706682	-1.244917	1.214166	0.1651				
O	-1.990514	-0.078414	-0.085434	0.1167				
H	-1.903035	-0.089111	0.866262					

PC3a

Geometry				Frequency (cm ⁻¹)				
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N	0.428560	0.230653	0.119434	52.5892	65.2286	89.5853	128.0114	157.7387
H	-1.501921	-0.047455	-0.178012	168.1555	370.0767	447.4967	677.8017	966.0204
C	1.392462	1.281933	0.174724	1002.8242	1058.6898	1068.9633	1267.6829	1274.4585
H	2.074022	1.222404	-0.674002	1455.7790	1476.6725	1519.6177	1531.8671	1545.8854
H	0.905166	2.246446	0.162156	1551.2842	1712.7750	3048.3784	3057.7845	3092.6379
H	2.002660	1.204914	1.074783	3100.5708	3192.6148	3199.2341	3788.2538	4033.0621
C	1.013755	-1.072289	0.160602	Rotational constants (cm ⁻¹) 0.3561 0.1010 0.0816				
H	0.242935	-1.826950	0.098585					
H	1.713229	-1.209632	-0.663978					
H	1.579572	-1.212643	1.081903					
O	-2.361177	-0.456851	-0.305959					
H	-2.808261	-0.366527	0.526284					

TS3b

Geometry

N	1.074110	0.474686	-0.307851
H	1.056880	0.537440	-1.306807
C	-0.088982	1.028691	0.269643
H	-0.012600	1.060170	1.350157
H	-0.295893	2.018186	-0.115192
H	-1.037591	0.398179	0.029376
C	1.403425	-0.858551	0.134294
H	2.291401	-1.205706	-0.376773
H	1.617501	-0.843849	1.197069
H	0.596533	-1.570383	-0.039171
O	-2.157099	-0.525272	-0.226058
H	-2.299413	-0.784656	0.685467

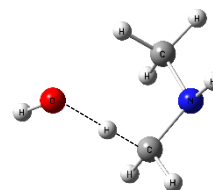
Frequency (cm⁻¹)

-506.1963i

85.3418	118.9968	137.0059	247.1843	373.6247
411.5201	706.9110	800.5595	995.1174	1078.2250
1108.1003	1172.0473	1244.7079	1321.6367	1394.6453
1485.3129	1505.1673	1514.3932	1539.9496	1557.5125
1575.9253	1615.4005	3063.4138	3131.9747	3141.9768
3188.3855	3200.4790	3678.1237	3909.5478	

Rotational constants (cm⁻¹)

0.3479
0.1209
0.0989



PC3b

Geometry

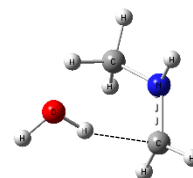
N	1.032980	0.434291	-0.326427
H	0.871120	0.452453	-1.312058
C	0.245642	1.284492	0.405719
H	0.387606	1.266881	1.470769
H	-0.011319	2.219291	-0.055181
H	-1.534690	0.019637	-0.001943
C	1.355354	-0.869528	0.197802
H	2.108469	-1.334615	-0.423776
H	1.765836	-0.760480	1.194273
H	0.486836	-1.520371	0.247620
O	-2.060126	-0.721409	-0.308018
H	-2.637316	-0.936006	0.414843

Frequency (cm⁻¹)

50.6324	83.2874	123.3622	146.6457	199.4303
293.4825	390.2495	410.2271	522.3436	666.5099
760.5821	999.8803	1084.6369	1190.0435	1299.0641
1352.1264	1503.2559	1530.1061	1541.3789	1562.4691
1602.4668	1695.3289	3095.1486	3160.1866	3193.0055
3209.9980	3319.4352	3712.3334	3812.1490	4030.1407

Rotational constants (cm⁻¹)

0.2899
0.1213
0.0951



Reaction 4 DMA + HO₂

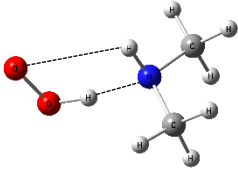
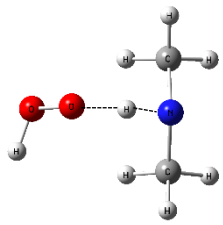
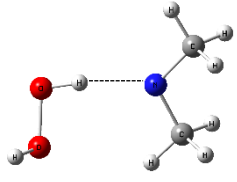
RC4

Geometry

C	1.516616	-1.199903	0.039407
N	0.758050	0.004836	-0.240078
C	1.489098	1.223702	0.051275
H	0.935203	-2.069221	-0.236522
H	1.722612	-1.257366	1.101222

Frequency (cm⁻¹)

15.1940	70.0903	81.3722	148.2541	225.5299
244.2189	354.6660	413.4849	899.3592	909.9315
972.1005	1077.8896	1140.4844	1217.6834	1260.5983
1286.1539	1317.5070	1502.1017	1528.7837	1533.3519
1544.8130	1556.5279	1571.4014	1573.8118	1712.9707

H	2.467466	-1.233362	-0.490341	3070.9657	3071.7635	3153.8974	3155.3618	3165.9709
H	0.470289	0.006299	-1.202303	3195.6984	3196.2665	3638.1921		
H	2.439095	1.283709	-0.477660	Rotational constants (cm⁻¹) 0.2508 0.0707 0.0619 				
H	0.888237	2.082227	-0.216657					
H	1.693434	1.275686	1.113693					
O	-2.352930	-0.026970	-0.520578					
O	-1.793430	-0.028117	0.656563					
H	-0.819756	-0.016423	0.461320					
TS4a								
Geometry				Frequency (cm ⁻¹)				
C	1.382972	-0.932894	0.416780	-2526.0067i				
N	0.962305	0.010199	-0.581698	38.9430	135.0665	147.2852	182.1421	215.9997
C	0.994702	1.366376	-0.116254	368.0512	413.1921	423.0644	627.3535	972.3052
H	1.321859	-1.937496	0.024152	1058.5291	1069.1164	1103.7318	1138.2636	1222.2044
H	0.765738	-0.867650	1.313090	1288.2030	1420.0035	1457.0646	1474.2988	1487.3075
H	2.410194	-0.724715	0.701679	1519.3234	1538.1853	1540.5921	1555.7164	1560.4006
H	-0.143583	-0.259839	-0.887435	3045.4751	3062.6074	3125.2254	3132.3738	3195.2865
H	2.016179	1.642597	0.128519	3203.9842	3919.7365	Rotational constants (cm⁻¹) 0.2278 0.0983 0.0855 		
H	0.628050	2.032478	-0.884689					
H	0.395862	1.498227	0.786940					
O	-1.353444	-0.478719	-0.812900					
O	-1.755857	-0.268658	0.491010					
H	-2.173728	0.588497	0.457801					
PC4a								
Geometry				Frequency (cm ⁻¹)				
C	1.223474	-0.976269	0.490817	27.0278	68.5335	73.7536	83.3561	124.8814
N	0.884405	0.356405	0.100333	169.1655	218.9813	260.6775	452.9739	750.2138
C	1.965566	1.278913	0.233169	968.3989	1017.0989	1055.2329	1058.6910	1070.9280
H	0.359446	-1.618584	0.408248	1270.2603	1275.8067	1425.4220	1456.9049	1477.8614
H	1.593951	-0.997953	1.515562	1519.1881	1532.2208	1545.7157	1553.5148	1629.6498
H	2.020916	-1.365503	-0.142298	3050.6637	3059.9626	3095.3313	3103.4688	3194.0859
H	-0.847309	0.499478	-0.578884	3210.6509	3620.9544	3957.5421	Rotational constants (cm⁻¹) 0.2756 0.0660 0.0553 	
H	2.814907	0.966394	-0.374153					
H	1.662042	2.269510	-0.074095					
H	2.313452	1.319898	1.265168					
O	-1.754308	0.391720	-0.902940					
O	-2.156304	-0.776412	-0.208520					
H	-2.807439	-0.430633	0.394037					
TS4b								
Geometry				Frequency (cm ⁻¹)				
C	1.650320	-0.884970	-0.337515	-1913.6544i				
N	1.228563	0.149062	0.577389	60.3224	102.2118	125.1028	188.3443	321.6479
C	0.579018	1.250104	0.029070	399.6025	452.5406	537.2621	596.5021	741.3089
H	2.184839	-1.652799	0.204881	1001.8147	1085.5078	1094.0287	1166.6347	1223.2608
H	2.324930	-0.460285	-1.070991	1284.6167	1323.1854	1360.3014	1444.2549	1504.2386
H	0.814115	-1.340367	-0.862204	1525.8319	1541.2592	1552.9206	1563.8669	1588.9356
H	0.756350	-0.219330	1.379408	3091.0914	3142.3360	3158.6966	3195.0661	3222.2432
H	-0.534160	0.871689	-0.449518	3688.2462	3921.2102	Rotational constants (cm ⁻¹)		
H	0.318909	1.998034	0.764795					

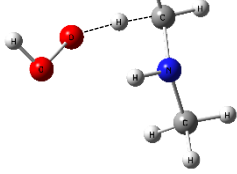
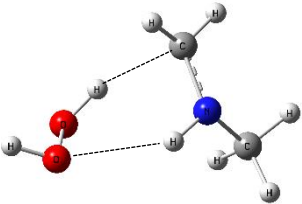
H	1.107898	1.671111	-0.815536	0.2403	
O	-1.608082	0.249238	-0.752454	0.0890	
O	-1.749597	-0.622046	0.313502	0.0782	
H	-2.388325	-0.185422	0.871546		
PC4b					
Geometry				Frequency (cm ⁻¹)	
C	1.820777	-0.835479	-0.413023	52.9704	73.8550 114.7221 141.0030 197.0459
N	1.229824	0.106937	0.502416	215.4599	258.5804 412.4698 417.1283 630.7558
C	0.860698	1.345103	0.049067	730.0590	790.4678 1002.7768 1055.5240 1087.4785
H	2.201518	-1.685780	0.136046	1186.2307	1300.8857 1357.1363 1424.7317 1504.1335
H	2.651812	-0.366296	-0.924761	1532.6994	1542.9585 1556.8392 1565.1714 1610.7213
H	1.113564	-1.191711	-1.158615	3084.3048	3158.0266 3196.0109 3209.4588 3316.9770
H	0.585093	-0.302364	1.148945	3658.0038	3698.1954 3952.8172
H	-0.977571	0.531606	-0.624934	Rotational constants (cm ⁻¹)	
H	0.400185	1.999308	0.765799	0.2356	
H	1.481426	1.784677	-0.709621	0.0776	
O	-1.713508	-0.095058	-0.643074	0.0709	
O	-1.769087	-0.508180	0.708943		
H	-2.579868	-0.105770	1.006390		

Table S2: MS-T factors for DMA + H/CH₃/OH/HO₂ reactions at 100-2000 K

T (K)	DMA	TS1a	TS1b	TS2a	TS2b	TS3a	TS3b	TS4a	TS4b
100	0.95	0.787	0.596	0.781	0.442	0.829	0.826	2.019	1.399
120	0.951	0.79	0.548	0.799	0.411	0.805	0.774	2.233	1.475
140	0.951	0.793	0.51	0.812	0.385	0.78	0.733	2.429	1.551
160	0.952	0.796	0.48	0.822	0.363	0.757	0.7	2.61	1.626
180	0.953	0.799	0.455	0.829	0.344	0.734	0.674	2.777	1.7
200	0.953	0.802	0.433	0.833	0.328	0.713	0.654	2.932	1.771
220	0.954	0.805	0.415	0.835	0.314	0.694	0.638	3.077	1.839
240	0.955	0.809	0.399	0.836	0.303	0.676	0.626	3.212	1.905
260	0.955	0.812	0.385	0.836	0.293	0.659	0.617	3.34	1.966
280	0.956	0.816	0.373	0.835	0.285	0.643	0.611	3.46	2.025
298	0.957	0.819	0.363	0.833	0.28	0.63	0.607	3.562	2.074
350	0.96	0.829	0.341	0.827	0.268	0.569	0.617	4.055	2.31
400	0.962	0.84	0.325	0.82	0.262	0.545	0.635	4.255	2.402
500	0.964	0.862	0.304	0.803	0.259	0.525	0.657	4.436	2.483
600	0.968	0.883	0.292	0.785	0.261	0.49	0.71	4.751	2.621
700	0.972	0.903	0.285	0.766	0.264	0.463	0.768	5.022	2.737
800	0.975	0.92	0.281	0.747	0.267	0.441	0.825	5.259	2.837
900	0.979	0.935	0.279	0.728	0.268	0.422	0.879	5.468	2.923
1000	0.983	0.947	0.278	0.709	0.269	0.407	0.928	5.653	2.998
1200	0.992	0.967	0.278	0.672	0.268	0.382	1.012	5.955	3.113
1400	1.001	0.98	0.279	0.638	0.264	0.364	1.076	6.17	3.185
1600	1.01	0.99	0.279	0.607	0.258	0.351	1.123	6.305	3.219
1800	1.021	0.997	0.279	0.579	0.25	0.341	1.155	6.369	3.221
2000	1.032	1.003	0.278	0.554	0.242	0.333	1.174	6.371	3.197

Table S3: The symmetry numbers (σ) of involved species for DMA + H/CH₃/OH/HO₂ reactions.

species	H	TS1a	TS1b	CH ₃	TS2a	TS2b
σ	1 (C ₁)	1 (C ₁)	1 (C ₁)	6 (D _{3h})	1 (C ₁)	1 (C ₁)

species	OH	RC3	TS3a	TS3b	HO ₂	RC4	TS4a	TS4b
σ	1 (C ₁)	1 (C ₁)	1 (C ₁)	1 (C ₁)	1 (C ₁)	1 (C ₁)	1 (C ₁)	1 (C ₁)

Table S4: “Projected” frequencies as a function of N—H bond distance (Å) for DMA + OH reaction calculated at BHandHLYP/cc-pVTZ level.

<i>R</i> (N-H)	2.1	2.3	2.5	2.7	2.9	3.1	3.3	3.5	3.7
DMA +	53.6325	47.7321	40.7286	36.2772	32.8593	30.1901	27.7897	25.3991	22.8301
OH	55.0295	64.2314	48.7231	46.8623	44.8253	43.0394	40.7996	38.4013	35.6929
	227.2063	232.2056	230.8528	231.4476	231.6373	231.7014	215.9777	189.6433	167.0356
vib	258.7020	260.3403	259.9144	260.3232	260.6048	247.8961	231.6465	208.1829	184.1649
(cm ⁻¹)	390.6652	391.1340	383.6618	330.9482	285.7151	260.3676	236.3864	231.4986	231.3612
	537.7518	444.3664	384.5711	363.9908	317.2332	274.1575	261.4348	261.2260	260.6272
	605.0747	526.8556	443.4883	399.3967	390.2310	387.4906	385.7973	384.9662	384.0554
	801.4280	782.4079	781.4953	776.7007	772.5266	769.7281	765.7933	765.4543	760.7389
	962.9757	963.8020	956.5410	953.2463	951.4540	950.4424	951.5638	951.1324	951.1152
	1074.8000	1075.2135	1074.1330	1073.9713	1073.8711	1073.8044	1073.7394	1073.6462	1073.6610
	1141.6560	1142.2221	1137.9205	1134.9258	1134.6379	1136.0560	1138.5134	1143.0450	1143.3276
	1147.2592	1149.4760	1142.3687	1142.6261	1142.8262	1143.0021	1143.1350	1143.3254	1143.7214
	1216.7827	1218.6937	1219.6995	1220.6141	1221.3291	1221.8771	1222.3091	1222.6610	1223.0338
	1318.1466	1318.2103	1316.8223	1315.9043	1315.1204	1314.7090	1314.7391	1313.9932	1314.4020
	1476.6405	1458.5909	1474.7113	1475.0539	1474.1133	1478.7011	1485.3731	1487.5198	1493.4923
	1500.5805	1500.8796	1499.8390	1499.4933	1499.1691	1498.8742	1498.5869	1498.5752	1498.1578
	1528.2139	1532.1676	1527.2684	1527.0295	1526.8470	1526.8583	1526.5490	1526.3875	1527.2653
	1532.5963	1533.0919	1532.9195	1533.0805	1533.1868	1533.2589	1533.2976	1533.4623	1533.3186
	1547.0135	1550.5737	1544.2995	1543.7380	1543.4020	1543.1689	1542.9861	1542.9681	1542.7822
	1562.4379	1555.8129	1561.4737	1560.8841	1559.8931	1559.7746	1560.5537	1560.5403	1560.2940
	1572.5369	1573.6893	1573.0478	1573.3077	1573.5205	1573.6842	1573.8010	1573.7621	1573.9818
	1572.9416	1607.3096	1575.1968	1576.3333	1576.5529	1577.0131	1578.9787	1580.8246	1579.1071
	3053.5196	3048.3806	3044.3687	3041.1130	3038.4473	3036.1923	3034.3237	3032.6895	3031.2271
	3056.5853	3051.7165	3047.7207	3044.6000	3042.0478	3039.8917	3038.1059	3036.5451	3035.1452
	3147.3770	3145.0119	3143.0151	3141.2237	3139.6590	3138.2537	3137.0056	3135.9260	3134.9088
	3148.3826	3146.5195	3143.3667	3141.4317	3139.7718	3138.2852	3137.0512	3136.0409	3135.0828
	3188.4936	3187.2501	3185.3131	3183.9447	3182.7254	3181.5970	3180.6049	3179.7477	3178.9400
	3188.8964	3188.1718	3185.8943	3184.5634	3183.3736	3182.2713	3181.3034	3180.4686	3179.6847
	3651.5564	3651.5603	3652.6078	3652.8634	3653.2138	3653.2980	3653.4028	3653.3272	3653.3356

<i>R</i> (N-H)	3.9	4.3	4.7	5.1	5.5	5.9	6.3	6.7	7.1
DMA +	19.2371	16.9898	13.4471	11.4222	10.1924	9.3748	8.7057	8.1968	7.7805
OH	35.0693	27.4049	24.2956	21.2522	19.1209	17.4524	16.0695	14.8986	13.8719
	144.6369	121.0104	101.1623	87.5632	77.1846	69.4567	62.9129	57.6628	53.3276
vib	171.4414	136.8300	117.2172	99.8380	86.5462	76.1659	67.6114	60.6361	54.7660
(cm ⁻¹)	231.1401	230.9773	231.0151	231.1476	231.2535	231.2934	231.3136	231.3190	231.3142

261.4859	259.3280	259.8115	259.5810	259.3668	259.0647	258.7280	258.6501	258.4404
383.5324	383.4334	382.7472	382.4437	382.8906	382.7087	382.1892	382.1212	381.9368
746.0982	759.5492	736.0475	725.2934	726.1747	724.4540	717.1882	715.7767	714.7358
955.4595	951.5254	954.5025	955.7059	953.5682	953.9722	953.6632	953.4115	953.5041
1073.6380	1073.5969	1073.6400	1073.6814	1073.7230	1073.7603	1073.8003	1073.8307	1073.8572
1143.2041	1139.5912	1141.9043	1142.0721	1140.7374	1138.1889	1141.8584	1143.6169	1143.8600
1143.3829	1143.5482	1143.7885	1144.3317	1143.8021	1143.8396	1143.9577	1147.5587	1148.8047
1223.2612	1223.8466	1224.3528	1224.7676	1225.0917	1225.3466	1225.5567	1225.7156	1225.8496
1317.3689	1314.8040	1317.8585	1317.4496	1317.2656	1317.1300	1317.1099	1317.0446	1317.1900
1487.2076	1477.9467	1475.2430	1473.3222	1469.8653	1474.8358	1477.5479	1481.0063	1490.2239
1498.0230	1497.7323	1497.6421	1497.5622	1497.6219	1497.4901	1497.5505	1497.4197	1498.0686
1527.9892	1526.3716	1527.9858	1531.6103	1529.7357	1531.5132	1531.5548	1532.3301	1532.9839
1533.2649	1533.2933	1533.2623	1533.2364	1533.3202	1533.1804	1533.1586	1534.3444	1535.1204
1542.5806	1542.6465	1542.5455	1542.5640	1542.5721	1542.6019	1542.5711	1542.5730	1542.6190
1552.0728	1558.2023	1553.6613	1556.0727	1557.5755	1558.2512	1559.6086	1559.4650	1559.9575
1573.9564	1574.0525	1574.0920	1574.1035	1574.1069	1574.1137	1574.1020	1574.0614	1574.0776
1584.4578	1576.4556	1581.9231	1583.1907	1582.6921	1583.8401	1581.7808	1581.3238	1585.4127
3030.0813	3028.1789	3026.8158	3025.8320	3025.0980	3024.5389	3024.0903	3023.7248	3023.4409
3034.0570	3032.2290	3030.9280	3029.9827	3029.3158	3028.7776	3028.4118	3028.1361	3027.8183
3134.1410	3132.9523	3132.1554	3131.7091	3131.4528	3131.3138	3131.2233	3131.1702	3131.1264
3134.4038	3133.2592	3132.5830	3132.1755	3132.0067	3131.8457	3131.7814	3131.7397	3131.7460
3178.4304	3177.4560	3176.9667	3176.6929	3176.5538	3176.4822	3176.4437	3176.4135	3176.3976
3179.3601	3178.2389	3178.0450	3177.8419	3177.8016	3177.8749	3177.7998	3177.6034	3177.5469
3653.1804	3653.4553	3653.7542	3654.2299	3654.5765	3654.9111	3655.1692	3655.4423	3655.5728

Table S5: “Projected” frequencies as a function of N—H bond distance (Å) for DMA + HO₂ reaction calculated at BHandHLYP/cc-pVTZ level.

<i>R</i> (N-H)	1.9	2.1	2.3	2.5	2.7	2.9	3.1	3.3	3.5
DMA +	15.7191	16.2593	16.1369	15.2772	14.2290	12.8136	11.8381	10.6282	9.5106
HO ₂	70.7594	70.6340	68.8289	64.3969	57.4991	51.2780	45.8820	41.2347	36.9990
vib	83.3958	78.5498	71.6439	65.5808	61.4895	56.9876	52.3575	47.8384	43.4762
(cm ⁻¹)	168.8997	152.4363	137.1531	123.2103	110.5630	99.1575	88.9037	79.7286	71.4520
	228.3149	230.5084	231.6764	232.0618	232.0215	231.7823	231.5282	231.3457	231.2592
	264.4069	264.6827	264.5145	264.1044	263.4174	262.6657	261.9842	261.4651	260.9934
	396.2219	393.8411	391.4744	389.3868	387.5500	386.0437	347.2834	305.7793	269.9283
	793.8840	687.4549	596.0200	518.5037	452.5241	396.0774	384.8294	383.8646	383.2864
	845.1998	832.7549	820.3363	810.7043	802.3534	795.5712	790.0381	785.5713	782.2915
	957.1967	957.8602	958.2954	958.4788	958.6562	958.5932	958.6787	958.9516	959.1813
	1076.2134	1075.3106	1074.7762	1074.3708	1074.0995	1073.9294	1073.8218	1073.7497	1073.6961
	1140.9280	1141.4197	1141.8714	1142.1984	1142.4567	1142.6676	1142.8410	1142.9861	1143.1067
	1199.3924	1196.8878	1193.9864	1192.1528	1190.8737	1189.8192	1189.1460	1188.1087	1187.8015
	1217.3044	1217.9507	1218.9524	1219.7564	1220.4345	1221.0190	1221.5068	1221.9062	1222.2558
	1278.6184	1272.9293	1268.4498	1264.8496	1261.9489	1259.5497	1257.6108	1255.9993	1254.7023
	1315.1227	1315.5669	1315.5393	1315.5205	1315.4440	1315.4507	1315.4311	1315.4655	1315.6134
	1501.7686	1501.2160	1500.6871	1500.1684	1499.7044	1499.3047	1498.9576	1498.6568	1498.3974
	1528.5753	1528.0902	1527.6742	1527.3004	1527.0162	1526.8042	1526.5724	1520.9439	1516.6370
	1532.6772	1532.7498	1532.9886	1533.1746	1533.2884	1533.3572	1527.7528	1526.5658	1526.4643
	1544.3231	1544.0113	1543.7605	1543.5368	1543.3278	1535.3717	1533.3947	1533.4216	1533.4342
	1553.2819	1552.2080	1551.4821	1549.6163	1543.9103	1543.1487	1543.0030	1542.8875	1542.7966

1570.2801	1570.0623	1569.2218	1564.1398	1555.9760	1553.2908	1552.2845	1551.7685	1551.3617
1573.2969	1573.2901	1573.4212	1573.5359	1572.3235	1571.7520	1571.5033	1571.3863	1571.3047
1656.3487	1618.7976	1590.6566	1575.1047	1573.6486	1573.7571	1573.8512	1573.9331	1574.0002
3063.8691	3057.3400	3051.8023	3047.3380	3043.7018	3040.6533	3038.1280	3035.9833	3034.1450
3066.0445	3059.9401	3054.7764	3050.5085	3046.9996	3044.1089	3041.6866	3039.6314	3037.8891
3151.3786	3148.4245	3145.7689	3143.4955	3141.5273	3139.8276	3138.3632	3137.0951	3135.9332
3151.8369	3148.8161	3146.1069	3143.7739	3141.7387	3139.9714	3138.4347	3137.0977	3136.0077
3193.2151	3190.8752	3188.6997	3186.7800	3185.0536	3183.5408	3182.2038	3181.0444	3180.0392
3193.7277	3191.3980	3189.2378	3187.3463	3185.6453	3184.1654	3182.8548	3181.7232	3180.7383
3317.2796	3456.2791	3546.2746	3609.1332	3647.3289	3651.0141	3651.5818	3651.6654	3651.4810
3643.7828	3647.1723	3649.4428	3651.1657	3658.2103	3681.7975	3707.6202	3719.6949	3727.9995

<i>R</i> (N-H)	3.9	4.3	4.7	5.1	5.5	5.9	6.3	6.7
DMA +	7.0938	5.2390	4.1845	4.6871	4.0984	4.2672	2.9567	3.7926
HO ₂	29.3563	23.2389	18.5970	15.1069	12.7698	11.1450	9.9994	8.8690
vib	35.4577	28.8495	23.8807	20.0368	17.1304	15.1414	13.9809	12.0315
(cm ⁻¹)	57.6585	47.0844	39.0670	32.8476	28.3337	24.7635	22.0652	19.5594
	211.9033	169.1630	137.7172	113.4281	96.3460	84.1788	77.6271	66.5279
	231.1870	231.1749	231.1498	231.0367	230.9590	230.8948	230.8569	230.8522
	260.1487	259.5088	258.9360	258.4680	258.0250	257.6964	257.1338	257.2144
	382.3347	381.9414	381.7538	381.9383	382.1490	381.8796	380.4083	382.2620
	776.3900	772.4497	769.3065	767.8243	764.4276	764.0404	760.6767	761.3308
	959.9632	960.5860	961.3240	961.6433	961.7010	962.9651	955.2252	963.5831
	1073.6297	1073.6110	1073.6191	1073.6378	1073.6642	1073.7154	1071.5549	1073.7835
	1143.2985	1143.4526	1143.5740	1143.6523	1143.7233	1143.7705	1142.3835	1143.8493
	1186.2027	1185.7501	1184.1049	1183.4957	1183.9038	1181.2986	1160.6835	1178.0335
	1222.9127	1223.5244	1224.0611	1224.5083	1224.8697	1225.1481	1225.7217	1225.5655
	1252.8066	1251.5249	1250.6246	1249.9028	1249.3356	1249.1531	1246.0262	1247.9177
	1315.8085	1316.0042	1316.1913	1316.4062	1316.6798	1316.5592	1316.9251	1317.1006
	1498.0046	1497.7670	1497.6334	1497.5219	1497.4892	1497.4418	1493.2903	1497.3992
	1510.4217	1506.5068	1504.4268	1503.2187	1502.6407	1501.3578	1503.4324	1503.1679
	1526.3100	1526.2028	1526.1096	1526.0434	1526.0021	1525.9507	1523.6041	1525.9160
	1533.4207	1533.3967	1533.3558	1533.2884	1533.2441	1533.2058	1526.8478	1533.1417
	1542.6805	1542.6299	1542.6090	1542.5895	1542.5858	1542.5799	1538.8330	1542.5613
	1550.8655	1550.5272	1550.2936	1550.1187	1549.9573	1549.7886	1550.9430	1549.9559
	1571.1980	1571.1050	1571.0295	1570.9185	1570.9348	1570.7320	1566.2172	1570.8515
	1574.1028	1574.1551	1574.1647	1574.1521	1574.1378	1574.1233	1571.4081	1574.1046
	3031.2362	3029.1251	3027.5816	3026.4545	3025.6307	3024.9590	2880.9158	3024.0579
	3035.1197	3033.0417	3031.6131	3030.5675	3029.7277	3029.1015	3024.4845	3028.3164
	3134.1199	3132.8917	3132.1164	3131.6418	3131.4401	3131.2476	3052.8718	3131.1014
	3134.3211	3133.1916	3132.4908	3132.0607	3131.8632	3131.7324	3131.2344	3131.5386
	3178.5122	3177.5219	3176.9512	3176.5995	3176.4971	3176.3733	3137.9094	3176.1165
	3179.2503	3178.2767	3177.7348	3177.4609	3177.3180	3177.2236	3176.5050	3177.0375
	3651.4978	3651.8165	3651.5917	3651.3575	3652.1473	3652.0203	3194.6029	3653.0501
	3749.3834	3763.9935	3767.7479	3789.0762	3800.9272	3756.7855	3654.8888	3784.9509

Table S6: Calculated rate constants ($\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$) for DMA + H reactions at temperature range of 100-2000 K.

T (K)	k_{1a}^{TST}	k_{1a}^{VTST}	$k_{1a}^{\text{MS-T}}$	k_{1b}^{TST}	k_{1b}^{VTST}	$k_{1b}^{\text{MS-T}}$
100	1.03759E8	9.21366E7	8.59562E7	2.19442E8	1.54043E8	1.37671E8
120	1.34953E8	1.205E8	1.12106E8	3.229E8	2.34015E8	1.86066E8
140	1.78191E8	1.60065E8	1.48586E8	4.8453E8	3.63187E8	2.59843E8
160	2.38712E8	2.15949E8	1.99595E8	7.38297E8	5.72993E8	3.72251E8
180	3.24104E8	2.95439E8	2.7173E8	1.13454E9	9.11731E8	5.41677E8
200	4.45206E8	4.08954E8	3.74665E8	1.74457E9	1.44829E9	7.92655E8
220	6.17255E8	5.71428E8	5.20849E8	2.66172E9	2.27632E9	1.15788E9
240	8.59942E8	8.02733E8	7.28474E8	4.00463E9	3.51444E9	1.67314E9
260	1.20018E9	1.12973E9	1.02047E9	5.913E9	5.30538E9	2.38378E9
280	1.67231E9	1.58499E9	1.42741E9	8.54522E9	7.81656E9	3.33407E9
298	2.2432E9	2.13962E9	1.91972E9	1.16887E10	1.08396E10	4.43365E9
350	5.02596E9	4.86397E9	4.34013E9	2.61897E10	2.50756E10	9.30279E9
400	1.0123E10	9.90017E9	8.83919E9	5.04644E10	4.93142E10	1.70488E10
500	3.27115E10	3.23923E10	2.92503E10	1.43504E11	1.43143E11	4.52545E10
600	8.23207E10	8.19594E10	7.50922E10	3.18744E11	3.18744E11	9.61502E10
700	1.72711E11	1.7235E11	1.60451E11	6.01899E11	5.99731E11	1.76483E11
800	3.17962E11	3.17721E11	3.00025E11	1.01531E12	1.00869E12	2.92617E11
900	5.31321E11	5.31321E11	5.07441E11	1.57837E12	1.56211E12	4.4981E11
1000	8.25014E11	8.25014E11	7.948E11	2.30703E12	2.27571E12	6.52445E11
1200	1.6964E12	1.6964E12	1.65365E12	4.30513E12	4.22805E12	1.20648E12
1400	3.00257E12	3.00257E12	2.93958E12	7.07585E12	6.93132E12	1.97219E12
1600	4.79291E12	4.79291E12	4.698E12	1.06589E13	1.0412E13	2.9444E12
1800	7.09994E12	7.09994E12	6.93304E12	1.5049E13	1.46816E13	4.11231E12
2000	9.94232E12	9.94232E12	9.66294E12	2.0258E13	1.97341E13	5.4571E12

Table S7: Calculated rate constants ($\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$) for DMA + CH_3 reactions at temperature range of 100-2000 K.

T (K)	k_{2a}^{TST}	$k_{2a}^{\text{MS-T}}$	k_{2b}^{TST}	$k_{2b}^{\text{MS-T}}$
100	410037.98	337094.38145	4617.6696	2148.43154
120	498862.48	419128.4138	6666.354	2881.04258
140	630503.4	538347.80315	9960.388	4032.33373
160	819594.2	707674.82395	15307.924	5836.95001
180	1.08757E6	946063.15089	24130.154	8710.15003
200	1.46816E6	1.2833E6	38932.23	13399.5503
220	2.01014E6	1.7594E6	64194.52	21129.01392
240	2.78698E6	2.4397E6	108094.9	34296.07822
260	3.90226E6	3.41601E6	184935.62	56739.41012
280	5.50712E6	4.81009E6	320189.74	95454.05429
298	7.53954E6	6.56263E6	527286.32	154273.94943
350	1.87947E7	1.61908E7	2.18117E6	608909.51167
400	4.4063E7	3.75589E7	7.76236E6	2.11407E6
500	2.04025E8	1.69951E8	6.64227E7	1.78459E7
600	7.30469E8	5.92374E8	3.55659E8	9.58957E7
700	2.10108E9	1.65579E9	1.35073E9	3.66866E8
800	5.09702E9	3.9051E9	4.01366E9	1.09913E9

900	1.08577E10	8.07393E9	9.97243E9	2.72994E9
1000	2.09024E10	1.50761E10	2.16491E10	5.92432E9
1200	6.19062E10	4.19364E10	7.64192E10	2.06455E10
1400	1.48262E11	9.44964E10	2.06374E11	5.44283E10
1600	3.05978E11	1.8389E11	4.64477E11	1.18649E11
1800	5.66188E11	3.2108E11	9.17753E11	2.24719E11
2000	9.64724E11	5.17885E11	1.64401E12	3.85513E11

Table S8: Calculated LPL (k^{LPL}), PEM (k^{PEM}), phenomenological rate constants (k_{H}), and overall rate constants (k) ($\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$) for DMA + OH reactions with MS-T anharmonicity correction at temperature range of 100-2000 K and pressure range of 0.001-100 atm.

T (K)	k_{3a}^{LPL}	k_{3a}^{PEM}	$k_{3a-\text{H}}^{0.001}$	$k_{3a}^{0.001}$	$k_{3a-\text{H}}^{10}$	k_{3a}^{10}	$k_{3a-\text{H}}^{100}$	k_{3a}^{100}
100	9.32902E13	1.55689E24	9.11504E13	9.11504E13	9.11809E13	9.11809E13	9.14131E13	9.14158E13
120	8.79541E13	8.58158E21	8.48915E13	8.48915E13	8.49231E13	8.49231E13	8.51749E13	8.51775E13
140	8.24729E13	2.2007E20	7.8447E13	7.8447E13	7.84786E13	7.84786E13	7.87345E13	7.87374E13
160	7.73679E13	1.46097E19	7.23385E13	7.23385E13	7.23686E13	7.23686E13	7.26186E13	7.26219E13
180	7.26536E13	1.8248E18	6.66264E13	6.66264E13	6.66552E13	6.66552E13	6.68922E13	6.68964E13
200	6.86192E13	3.60124E17	6.15989E13	6.15989E13	6.1625E13	6.1625E13	6.18503E13	6.18503E13
220	6.50687E13	9.58995E16	5.7104E13	5.7104E13	5.71281E13	5.71281E13	5.73361E13	5.73361E13
240	6.19113E13	3.26277E16	5.3071E13	5.3071E13	5.30931E13	5.30931E13	5.32828E13	5.32828E13
260	5.91269E13	1.32903E16	4.95032E13	4.95032E13	4.95231E13	4.95231E13	4.96956E13	4.96956E13
280	5.65081E13	6.27737E15	4.6243E13	4.6243E13	4.62608E13	4.62608E13	4.64159E13	4.64159E13
298	5.43144E13	3.47226E15	4.3623E13	4.3623E13	4.36393E13	4.36393E13	4.37804E13	4.37804E13
350	4.60144E13	8.96666E14	3.55276E13	3.55276E13	3.5539E13	3.5539E13	3.56391E13	3.56391E13
400	4.05723E13	3.64666E14	3.10372E13	3.10372E13	3.10456E13	3.10456E13	3.112E13	3.112E13
500	3.12752E13	1.18052E14	2.52301E13	2.52301E13	2.52347E13	2.52347E13	2.52755E13	2.52755E13
600	2.29041E13	5.878E13	2.00734E13	2.00734E13	2.00757E13	2.00757E13	2.0096E13	2.0096E13
700	1.75552E13	3.7773E13	1.64197E13	1.64197E13	1.64209E13	1.64209E13	1.64306E13	1.64306E13
800	1.42629E13	2.83011E13	1.38709E13	1.38709E13	1.38715E13	1.38715E13	1.38761E13	1.38761E13
900	1.22172E13	2.34276E13	1.21002E13	1.21002E13	1.21004E13	1.21004E13	1.21025E13	1.21025E13
1000	1.09732E13	2.07835E13	1.09527E13	1.09527E13	1.09528E13	1.09528E13	1.09538E13	1.09538E13
1200	9.71432E12	1.84436E13	9.72744E12	9.72744E12	9.72746E12	9.72746E12	9.72765E12	9.72765E12
1400	9.39519E12	1.81453E13	9.37093E12	9.37093E12	9.37093E12	9.37093E12	9.37098E12	9.37098E12
1600	9.53687E12	1.87136E13	9.49442E12	9.49442E12	9.49442E12	9.49442E12	9.49444E12	9.49444E12
1800	9.98518E12	1.99183E13	9.88664E12	9.88664E12	9.88664E12	9.88664E12	9.88664E12	9.88664E12
2000	1.06508E13	2.15479E13	1.04715E13	1.04715E13	1.04715E13	1.04715E13	1.04715E13	1.04715E13

T (K)	k_{3b}^{LPL}	k_{3b}^{PEM}	$k_{3b-\text{H}}^{0.001}$	$k_{3b}^{0.001}$	$k_{3b-\text{H}}^{10}$	k_{3b}^{10}	$k_{3b-\text{H}}^{100}$	k_{3b}^{100}
100	9.29427E13	8.7017E17	4.54941E13	4.54941E13	3.9678E13	6.08467E13	1.07414E13	8.24226E13
120	8.43511E13	3.30375E16	3.47043E13	3.47043E13	3.26563E13	4.63159E13	1.10368E13	6.85735E13
140	7.60414E13	4.03116E15	2.68762E13	2.68762E13	2.65534E13	3.53493E13	1.09244E13	5.60993E13
160	6.63886E13	9.2152E14	2.11341E13	2.11341E13	2.15273E13	2.72123E13	1.04856E13	4.5308E13
180	5.48719E13	3.09057E14	1.69348E13	1.69348E13	1.75612E13	2.12856E13	9.85324E12	3.64275E13
200	4.28084E13	1.33778E14	1.38497E13	1.38497E13	1.44924E13	1.69836E13	9.13078E12	2.93426E13
220	3.20612E13	6.90397E13	1.15161E13	1.15161E13	1.20824E13	1.37882E13	8.34962E12	2.36968E13
240	2.37845E13	4.05927E13	9.74441E12	9.74441E12	1.02104E13	1.14089E13	7.58593E12	1.92908E13

260	1.78798E13	2.63536E13	8.38607E12	8.38607E12	8.75502E12	9.61906E12	6.87914E12	1.58766E13
280	1.37664E13	1.84554E13	7.32167E12	7.32167E12	7.60702E12	8.24437E12	6.23981E12	1.32194E13
298	1.11401E13	1.40932E13	6.5516E12	6.5516E12	6.7744E12	7.26839E12	5.72638E12	1.11401E13
350	7.01455E12	8.09404E12	5.13554E12	5.13554E12	5.24387E12	5.50431E12	4.70241E12	7.01455E12
400	5.2079E12	5.77316E12	4.34104E12	4.34104E12	4.50565E12	4.50565E12	4.0796E12	5.2079E12
500	3.63944E12	3.90646E12	3.43336E12	3.43336E12	3.47972E12	3.47972E12	3.5512E12	3.63944E12
600	3.2522E12	3.45909E12	3.19732E12	3.19732E12	3.21174E12	3.21174E12	3.23139E12	3.2522E12
700	3.25344E12	3.46037E12	3.2375E12	3.2375E12	3.24218E12	3.24218E12	3.24807E12	3.24807E12
800	3.45103E12	3.68761E12	3.44262E12	3.44262E12	3.44419E12	3.44419E12	3.44608E12	3.44608E12
900	3.7697E12	4.05729E12	3.75939E12	3.75939E12	3.75993E12	3.75993E12	3.76057E12	3.76057E12
1000	4.17784E12	4.53531E12	4.16265E12	4.16265E12	4.16284E12	4.16284E12	4.16307E12	4.16307E12
1200	5.21049E12	5.7627E12	5.17992E12	5.17992E12	5.17995E12	5.17995E12	5.18E12	5.18E12
1400	6.47869E12	7.29986E12	6.42096E12	6.42096E12	6.42096E12	6.42096E12	6.42098E12	6.42098E12
1600	7.95259E12	9.11795E12	7.84775E12	7.84775E12	7.84775E12	7.84775E12	7.84782E12	7.84782E12
1800	9.58676E12	1.1165E13	9.40513E12	9.40513E12	9.40513E12	9.40513E12	9.40513E12	9.40513E12
2000	1.13686E13	1.34239E13	1.10698E13	1.10698E13	1.10698E13	1.10698E13	1.10698E13	1.10698E13

Table S9: Calculated LPL (k^{LPL}), phenomenological rate constants (k_{H}), overall rate constants (k), and the case without the consideration of RC ($k_{\text{out}}^{\text{RC}}$) ($\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$) for DMA + HO₂ reactions with MS-T anharmonicity correction at temperature range of 100-2000 K and pressure range of 0.001-100 atm.

T (K)	k_{4a}^{LPL}	$k_{4a,\text{out}}^{\text{RC}}$	$k_{4a-\text{H}}^{0.001}$	$k_{4a}^{0.001}$	$k_{4a-\text{H}}^{10}$	k_{4a}^{10}	$k_{4a-\text{H}}^{100}$	k_{4a}^{100}
100	8.09121E5	7.81082E-7	3.18231E5	4.52939E12	7.113E4	1.40865E14	816.76541	1.46224E14
120	6.56992E5	2.43773E-4	3.03247E5	2.69568E12	1.7339E4	1.63048E14	2276.56591	1.75776E14
140	3.93045E5	0.01592	3.02043E5	1.63324E12	3.6376E4	1.76103E14	5708.31538	2.00382E14
160	3.62786E5	0.38963	3.15525E5	1.0076E12	6.7731E4	1.79674E14	13094.44346	2.19088E14
180	3.71364E5	4.94674	3.45753E5	6.33939E11	1.15110E5	1.75071E14	27798.41486	2.31718E14
200	4.11118E5	39.61134	3.96493E5	4.06718E11	1.83030E5	1.64633E14	5.5166E5	2.38835E14
220	4.85310E5	226.27981	4.72514E5	2.65522E11	2.76978E5	1.50172E14	1.02951E5	2.40381E14
240	5.87614E5	1000.755	5.82509E5	1.76005E11	4.05284E5	1.33693E14	1.82202E5	2.37072E14
260	7.44505E5	3637.27539	7.40346E5	1.18533E11	5.81176E5	1.16899E14	3.08761E5	2.29989E14
280	9.67741E5	11281.14614	9.63116E5	8.0714E10	8.21747E5	1.00427E14	5.03257E5	2.19158E14
298	1.24122E6	28017.71682	1.24182E6	5.77806E10	1.11572E6	8.66306E13	7.60360E5	2.07165E14
350	2.93115E6	264287.0749	2.93402E6	2.42346E10	2.84143E6	5.7054E13	2.38953E6	1.75267E14
400	6.63015E6	1.38053E6	6.6407E6	1.05029E10	6.57792E6	3.44422E13	6.11208E6	1.30748E14
500	3.25607E7	1.62748E7	3.262E7	3.262E7	3.25914E7	1.21158E13	3.22007E7	6.4142E13
600	1.41442E8	1.03063E8	1.41719E8	1.41719E8	1.41719E8	1.41719E8	1.41719E8	1.41719E8
700	4.98285E8	4.33413E8	4.99188E8	4.99188E8	4.99188E8	4.99188E8	4.99188E8	4.99188E8
800	1.45794E9	1.38924E9	1.45985E9	1.45985E9	1.45985E9	1.45985E9	1.45985E9	1.45985E9
900	3.65793E9	3.66281E9	3.65871E9	3.65871E9	3.65871E9	3.65871E9	3.65871E9	3.65871E9
1000	8.11724E9	8.35995E9	8.10388E9	8.10388E9	8.10388E9	8.10388E9	8.10388E9	8.10388E9
1200	3.01765E10	3.19026E10	2.99306E10	2.99306E10	2.99306E10	2.99306E10	2.99306E10	2.99306E10
1400	8.53909E10	9.1052E10	8.37849E10	8.37849E10	8.37849E10	8.37849E10	8.37849E10	8.37849E10
1600	1.99062E11	2.12587E11	1.92392E11	1.92392E11	1.92392E11	1.92392E11	1.92392E11	1.92392E11
1800	4.01269E11	4.28244E11	3.80562E11	3.80562E11	3.80562E11	3.80562E11	3.80562E11	3.80562E11
2000	7.24777E11	7.71784E11	6.72419E11	6.72419E11	6.72419E11	6.72419E11	6.72423E11	6.72423E11

T (K)	k_{4b}^{LPL}	$k_{4b,out}^{RC}$	$k_{4b-H}^{0.001}$	$k_{4b}^{0.001}$	k_{4b-H}^{10}	k_{4b}^{10}	k_{4b-H}^{100}	k_{4b}^{100}
100	8225.87757	2.09999E-5	3692.70435	3.13849E12	4929.06269	9.76334E13	11.97711	1.01347E14
120	5312.33187	0.00191	3574.04196	1.78052E12	11453.31684	1.07657E14	35.95403	1.16064E14
140	4474.20161	0.05305	3732.20864	1.04287E12	23227.93074	1.12445E14	99.32645	1.27948E14
160	4591.35225	0.70229	4207.80831	6.27764E11	42196.16033	1.11937E14	255.00366	1.36494E14
180	5287.43603	5.6816	5115.12282	3.88039E11	70467.25763	1.07213E14	612.61439	1.41896E14
200	6733.08104	32.54324	6664.48216	2.45661E11	110554.80902	9.94587E13	1384.68808	1.44281E14
220	9221.3429	144.52516	9218.25579	1.58703E11	165538.76936	8.97538E13	2957.65805	1.43666E14
240	13425.94811	529.74998	13449.28288	1.04409E11	240369.5488	7.93066E13	6024.41047	1.4062E14
260	20407.15124	1669.8924	20513.27068	6.98031E10	342093.6369	6.88183E13	11789.20482	1.35374E14
280	32208.09638	4663.52247	32401.78674	4.72766E10	480935.95922	5.88068E13	22306.07697	1.28308E14
298	49637.40426	10769.53085	49965.55944	3.36108E10	649634.23181	5.04474E13	38630.53686	1.20647E14
350	192188.76683	88681.4775	193525.58899	1.37952E10	1.61867E6	3.249E13	178255.56595	9.98338E13
400	655998.53839	438907.27272	660586.2697	5.9246E9	3.71331E6	1.94408E13	643201.3917	7.38062E13
500	5.57842E6	5.07055E6	5.61727E6	5.61727E6	1.82427E7	6.78165E12	5.59883E6	3.59043E13
600	3.21432E7	3.23174E7	3.23617E7	3.23617E7	7.81824E7	3.23617E7	3.23617E7	3.23617E7
700	1.32015E8	1.3786E8	1.32859E8	1.32859E8	2.72058E8	1.32859E8	1.32859E8	1.32859E8
800	4.22373E8	4.47524E8	4.24726E8	4.24726E8	7.87527E8	4.24726E8	4.24726E8	4.24726E8
900	1.11918E9	1.19225E9	1.12385E9	1.12385E9	1.95582E9	1.12385E9	1.12385E9	1.12385E9
1000	2.57122E9	2.74207E9	2.57648E9	2.57648E9	4.2978E9	2.57648E9	2.57648E9	2.57648E9
1200	9.90676E9	1.05298E10	9.85791E9	9.85791E9	1.56463E10	9.85791E9	9.85791E9	9.85791E9
1400	2.83924E10	3.00443E10	2.79414E10	2.79414E10	4.32504E10	2.79414E10	2.79414E10	2.79414E10
1600	6.6307E10	6.98045E10	6.42741E10	6.42741E10	9.82252E10	6.42741E10	6.42741E10	6.42741E10
1800	1.33206E11	1.39673E11	1.26722E11	1.26722E11	1.92462E11	1.26722E11	1.26722E11	1.26722E11
2000	2.39267E11	2.49982E11	2.2273E11	2.2273E11	3.37423E11	2.2273E11	2.2273E11	2.2273E11

Table S10: All the calculated phenomenological rate constants ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) for DMA + OH reactions at temperature range of 100-2000 K and pressure range of 0.001-100 atm.

0.001 atm

T (K)	R->W	R->Pa	R->Pb	R->	W->R	W->Pa	W->Pb	W->
100	1.44844e-21	1.73455e-10	8.68876e-11	2.60343E-10	2.7844e-11	***	8223.3	8223.3
120	8.95125e-21	1.66536e-10	7.08079e-11	2.37344E-10	4.71561e-08	***	40090.3	40090.3
140	2.90209e-20	1.58826e-10	5.79033e-11	2.16729E-10	8.55008e-06	***	100566	100566
160	6.11699e-20	1.51067e-10	4.7729e-11	1.98796E-10	0.000376418	***	186497	186497
180	1.03358e-19	1.43649e-10	3.97624e-11	1.83411E-10	0.00692555	***	293693	293693
200	1.53138e-19	1.36721e-10	3.35132e-11	1.70234E-10	0.071578	***	423746	423746
220	***	1.30351e-10	2.85952e-11	1.58946E-10	***	***	***	***
240	***	1.24501e-10	2.46856e-11	1.49187E-10	***	***	***	***
260	***	1.19127e-10	2.15544e-11	1.40681E-10	***	***	***	***
280	***	1.1417e-10	1.90233e-11	1.33193E-10	***	***	***	***
298	***	1.10039e-10	1.71526e-11	1.27192E-10	***	***	***	***
350	***	9.95368e-11	1.32688e-11	1.12806E-10	***	***	***	***
400	***	9.09747e-11	1.09208e-11	1.01895E-10	***	***	***	***
500	***	7.69301e-11	8.36548e-12	8.52956E-11	***	***	***	***
600	***	6.58505e-11	7.23874e-12	7.30892E-11	***	***	***	***
700	***	5.72415e-11	6.80415e-12	6.40456E-11	***	***	***	***
800	***	5.0925e-11	6.75615e-12	5.76812E-11	***	***	***	***
900	***	4.66145e-11	6.95298e-12	5.35675E-11	***	***	***	***
1000	***	4.3928e-11	7.32208e-12	5.12501E-11	***	***	***	***
1200	***	4.19475e-11	8.43167e-12	5.03792E-11	***	***	***	***
1400	***	4.27932e-11	9.9193e-12	5.27125E-11	***	***	***	***
1600	***	4.53672e-11	1.17205e-11	5.70877E-11	***	***	***	***
1800	***	4.91563e-11	1.3806e-11	6.29623E-11	***	***	***	***
2000	***	5.38896e-11	1.61589e-11	7.00485E-11	***	***	***	***

1 atm

T (K)	R->W	R->Pa	R->Pb	R->	W->R	W->Pa	W->Pb	W->
100	6.31011e-13	1.73461e-10	9.13802e-11	2.65472E-10	0.0114667	***	24706.6	24706.6
120	4.16565e-13	1.66542e-10	7.41388e-11	2.41097E-10	2.07774	***	261871	261873
140	2.79425e-13	1.58832e-10	6.03179e-11	2.19429E-10	77.5439	***	1.48151e+06	1.48159e+06
160	1.90741e-13	1.51073e-10	4.94676e-11	2.00731E-10	1082	***	5.41745e+06	5.41853e+06
180	1.33226e-13	1.43655e-10	4.10169e-11	1.84805E-10	7915.03	***	1.44078e+07	1.44157e+07
200	9.56537e-14	1.36727e-10	3.44239e-11	1.71247E-10	37325.6	***	3.05328e+07	3.05702e+07
220	7.09618e-14	1.30356e-10	2.92614e-11	1.59688E-10	130037	***	5.52622e+07	5.53923e+07
240	5.40334e-14	1.24506e-10	2.51767e-11	1.49737E-10	362685	***	8.90392e+07	8.94019e+07
260	4.2052e-14	1.19132e-10	2.1919e-11	1.41093E-10	856921	***	1.31728e+08	1.32585e+08
280	3.33288e-14	1.14174e-10	1.92961e-11	1.33503E-10	1.78424e+06	***	1.82902e+08	1.84686e+08
298	2.74561e-14	1.10043e-10	1.73638e-11	1.27434E-10	3.18209e+06	***	2.36199e+08	2.39381e+08
350	***	9.954e-11	1.33881e-11	1.12928E-10	***	***	***	***
400	***	9.09771e-11	1.09841e-11	1.01961E-10	***	***	***	***
500	***	7.69315e-11	8.3843e-12	8.53158E-11	***	***	***	***
600	***	6.58512e-11	7.24461e-12	7.30958E-11	***	***	***	***
700	***	5.72419e-11	6.80603e-12	6.40479E-11	***	***	***	***

800	***	5.09252e-11	6.75677e-12	5.7682E-11	***	***	***	***
900	***	4.66146e-11	6.95319e-12	5.35678E-11	***	***	***	***
1000	***	4.3928e-11	7.32216e-12	5.12502E-11	***	***	***	***
1200	***	4.19475e-11	8.43168e-12	5.03792E-11	***	***	***	***
1400	***	4.27932e-11	9.9193e-12	5.27125E-11	***	***	***	***
1600	***	4.53672e-11	1.17205e-11	5.70877E-11	***	***	***	***
1800	***	4.91563e-11	1.3806e-11	6.29623E-11	***	***	***	***
2000	***	5.38896e-11	1.61589e-11	7.00485E-11	***	***	***	***

10 atm

T (K)	R->W	R->Pa	R->Pb	R->	W->R	W->P1	W->P2	W->
100	4.04293e-11	1.73513e-10	7.57797e-11	2.89722E-10	0.734634	3.00448e+10	26495.8	3.00448e+10
120	2.787e-11	1.66598e-10	6.66294e-11	2.61097E-10	138.984	***	318561	318700
140	1.89503e-11	1.5889e-10	5.72079e-11	2.35048E-10	5256.03	***	2.14547e+06	2.15073e+06
160	1.28391e-11	1.5113e-10	4.86169e-11	2.12586E-10	72708.5	***	9.44764e+06	9.52035e+06
180	8.74459e-12	1.43711e-10	4.12332e-11	1.93689E-10	517092	***	2.99331e+07	3.04502e+07
200	6.02819e-12	1.36779e-10	3.50683e-11	1.77875E-10	2.32538e+06	***	7.37735e+07	7.60989e+07
220	4.23563e-12	1.30406e-10	3.00013e-11	1.64643E-10	7.57491e+06	***	1.50596e+08	1.58171e+08
240	3.03642e-12	1.24553e-10	2.5866e-11	1.53455E-10	1.95172e+07	***	2.66539e+08	2.86057e+08
260	2.2208e-12	1.19175e-10	2.25027e-11	1.43899E-10	4.22817e+07	***	4.23496e+08	4.65778e+08
280	1.65605e-12	1.14214e-10	1.97647e-11	1.35635E-10	8.04342e+07	***	6.19989e+08	7.00423e+08
298	1.29325e-12	1.1008e-10	1.77359e-11	1.29109E-10	1.3197e+08	***	8.28503e+08	9.60472e+08
350	6.7285e-13	9.95687e-11	1.35487e-11	1.1379E-10	3.99017e+08	***	1.55772e+09	1.95674e+09
400	***	9.09994e-11	1.13349e-11	1.02334E-10	***	***	***	***
500	***	7.69442e-11	8.47842e-12	8.54226E-11	***	***	***	***
600	***	6.5858e-11	7.27138e-12	7.31294E-11	***	***	***	***
700	***	5.72454e-11	6.81398e-12	6.40594E-11	***	***	***	***
800	***	5.09269e-11	6.75922e-12	5.76861E-11	***	***	***	***
900	***	4.66154e-11	6.95397e-12	5.35694E-11	***	***	***	***
1000	***	4.39284e-11	7.32242e-12	5.12508E-11	***	***	***	***
1200	***	4.19476e-11	8.43171e-12	5.03793E-11	***	***	***	***
1400	***	4.27932e-11	9.9193e-12	5.27125E-11	***	***	***	***
1600	***	4.53672e-11	1.17205e-11	5.70877E-11	***	***	***	***
1800	***	4.91563e-11	1.3806e-11	6.29623E-11	***	***	***	***
2000	***	5.38896e-11	1.61589e-11	7.00485E-11	***	***	***	***

100 atm

T (K)	R->W	R->Pa	R->Pb	R->	W->R	W->P1	W->P2	W->
100	1.36901e-10	1.73955e-10	2.05147e-11	3.31371E-10	2.48761	4.58876e+10	26804.9	4.58876E10
120	1.17394e-10	1.67092e-10	2.25186e-11	3.07005E-10	585.42	6.56883e+10	332309	6.56886E10
140	9.73269e-11	1.59408e-10	2.3536e-11	2.80271E-10	26993.6	8.84775e+10	2.3715e+06	8.84799E10
160	7.86426e-11	1.51652e-10	2.36805e-11	2.53975E-10	445293	1.11743e+11	1.13291e+07	1.11755E11
180	6.23956e-11	1.44222e-10	2.31351e-11	2.29753E-10	3.68742e+06	1.37501e+11	3.95281e+07	1.37544E11
200	4.8908e-11	1.37279e-10	2.20944e-11	2.08281E-10	1.88281e+07	***	1.0773e+08	1.26558E8
220	3.81078e-11	1.30881e-10	2.07326e-11	1.89721E-10	6.77673e+07	***	2.41634e+08	3.09401E8
240	2.9652e-11	1.24998e-10	1.92175e-11	1.73868E-10	1.88217e+08	***	4.64542e+08	6.5276E8
260	2.31257e-11	1.1959e-10	1.76812e-11	1.60397E-10	4.30043e+08	***	7.90767e+08	1.22081E9
280	1.81344e-11	1.14597e-10	1.62124e-11	1.48944E-10	8.47222e+08	***	1.22345e+09	2.07067E9

298	1.46726e-11	1.10436e-10	1.49921e-11	1.40101E-10	1.41542e+09	***	1.69964e+09	3.11506E9
350	8.23514e-12	9.98493e-11	1.21497e-11	1.20234E-10	4.33425e+09	***	3.44281e+09	7.77706E9
400	4.93902e-12	9.12173e-11	1.02631e-11	1.06419E-10	9.19516e+09	***	5.45734e+09	1.46525E10
500	***	7.70684e-11	8.65258e-12	8.5721E-11	***	***	***	***
600	***	6.59247e-11	7.31587e-12	7.32406E-11	***	***	***	***
700	***	5.72795e-11	6.82637e-12	6.41059E-11	***	***	***	***
800	***	5.09438e-11	6.76293e-12	5.77067E-11	***	***	***	***
900	***	4.66235e-11	6.95516e-12	5.35787E-11	***	***	***	***
1000	***	4.39322e-11	7.32283e-12	5.1255E-11	***	***	***	***
1200	***	4.19484e-11	8.43179e-12	5.03802E-11	***	***	***	***
1400	***	4.27934e-11	9.91933e-12	5.27127E-11	***	***	***	***
1600	***	4.53673e-11	1.17206e-11	5.70879E-11	***	***	***	***
1800	***	4.91563e-11	1.3806e-11	6.29623E-11	***	***	***	***
2000	***	5.38896e-11	1.61589e-11	7.00485E-11	***	***	***	***

Table S11: All the calculated phenomenological rate constants ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) for DMA + HO₂ reactions at temperature range of 100-2000 K and pressure range of 0.001-100 atm.

0.001 atm

T (K)	R->W	R->Pa	R->Pb	R->	W->R	W->Pa	W->Pb	W->
100	7.07809E-12	5.89794e-38	4.16399e-21	7.07809E-12	5.46735E-12	3.20047e-43	3.88464e-21	5.46735E-12
120	3.81274E-12	4.49562e-34	3.82655e-21	3.81274E-12	5.73134E-8	1.14059e-36	2.69226e-17	5.73134E-8
140	2.12369E-12	2.74484e-31	3.80009e-21	2.12369E-12	3.61477E-5	2.87756e-32	1.29154e-14	3.61477E-5
160	1.22064E-12	3.46324e-29	4.09102e-21	1.22064E-12	0.00398	2.21346e-28	1.16656e-12	0.00398
180	7.22488E-13	1.52825e-27	4.76167e-21	7.22488E-13	0.13767	5.49494e-26	3.47103e-11	0.13767
200	4.39042E-13	3.23244e-26	5.95525e-21	4.39042E-13	2.13618	1.12682e-23	4.76544e-10	2.13618
220	2.73416E-13	4.00369e-25	7.94099e-21	2.73416E-13	18.60261	4.00599e-22	3.74544e-09	18.60261
240	1.73815E-13	3.31844e-24	1.11961e-20	1.73815E-13	105.3041	6.65546e-21	1.93999e-08	105.3041
260	1.12586E-13	2.01851e-23	1.65468e-20	1.12586E-13	429.614	1.5112e-19	7.31869e-08	429.614
280	7.40955E-14	9.62411e-23	2.54016e-20	7.40955E-14	1357.344	8.6173e-19	2.15511e-07	1357.344
298	5.15318E-14	3.3181e-22	3.82854e-20	5.15318E-14	3216.56	1.04249e-17	4.8117e-07	3216.56
350	1.90464E-14	6.08516e-21	1.33554e-19	1.90465E-14	19785.98	2.74445e-16	2.55086e-06	19785.98
400	7.88046E-15	5.17089e-20	4.3933e-19	7.88095E-15	61072	1.04353e-15	6.96272e-06	61072
500	***	1.16401e-18	3.62147e-18	4.78548E-18	***	***	***	***
600	***	1.04194e-17	1.98472e-17	3.02666E-17	***	***	***	***
700	***	5.43262e-17	7.83505e-17	1.32677E-16	***	***	***	***
800	***	2.00096e-16	2.42389e-16	4.42485E-16	***	***	***	***
900	***	5.80355e-16	6.25061e-16	1.20542E-15	***	***	***	***
1000	***	1.41614e-15	1.40284e-15	2.81898E-15	***	***	***	***
1200	***	5.87831e-15	5.21647e-15	1.10948E-14	***	***	***	***
1400	***	1.76015e-14	1.45825e-14	3.2184E-14	***	***	***	***
1600	***	4.23665e-14	3.34885e-14	7.5855E-14	***	***	***	***
1800	***	8.73309e-14	6.67029e-14	1.54034E-13	***	***	***	***
2000	***	1.60466e-13	1.19392e-13	2.79858E-13	***	***	***	***

1 atm

T (K)	R->W	R->Pa	R->Pb	R->	W->R	W->Pa	W->Pb	W->
100	1.78133E-10	5.89794e-38	6.09882e-22	1.78133E-10	1.37589E-10	5.08171e-44	6.62961e-21	1.37589E-10
120	1.63089E-10	4.49562e-34	1.07465e-21	1.63089E-10	2.45131E-6	3.64614e-37	6.82821e-17	2.45131E-6
140	1.40023E-10	2.74484e-31	1.68574e-21	1.40023E-10	0.00238	6.58502e-32	4.88952e-14	0.00238
160	1.14981E-10	3.46324e-29	2.47725e-21	1.14981E-10	0.37437	9.24224e-28	6.42048e-12	0.37437
180	9.15801E-11	1.52825e-27	3.53546e-21	9.15801E-11	17.44071	1.02156e-25	2.68213e-10	17.44071
200	7.14615E-11	3.23244e-26	5.02558e-21	7.14615E-11	347.41	9.47609e-25	4.99572e-09	347.41
220	5.50077E-11	4.00369e-25	7.23637e-21	5.50077E-11	3737.31	6.80872e-22	5.16127e-08	3737.31
240	4.1954E-11	3.31844e-24	1.06615e-20	4.1954E-11	25365.4	1.97916e-21	3.42544e-07	25365.4
260	3.18195E-11	2.01851e-23	1.61404e-20	3.18195E-11	121042.4	2.42862e-19	1.61882e-06	121042.4
280	2.40376E-11	9.62411e-23	2.5092e-20	2.40376E-11	438357	1.27551e-17	5.86141e-06	438357.0
298	1.86493E-11	3.3181e-22	3.80422e-20	1.86493E-11	1.15657E6	2.38474e-16	1.55587e-05	1.15657E6
350	8.92173E-12	6.08516e-21	1.33431e-19	8.92173E-12	9.12349E6	2.12091e-13	0.000128586	9.12349E6
400	4.44118E-12	5.17089e-20	4.39263e-19	4.44118E-12	3.32574E7	2.8881e-11	0.000506415	3.32574E7
500	1.20972E-12	1.16401e-18	3.62145e-18	1.20973E-12	1.56147E8	2.82533e-08	0.00302345	1.56147E8
600	***	1.04194e-17	1.98472e-17	3.02666E-17	***	***	***	***
700	***	5.43262e-17	7.83505e-17	1.32677E-16	***	***	***	***
800	***	2.00096e-16	2.42389e-16	4.42485E-16	***	***	***	***
900	***	5.80355e-16	6.25061e-16	1.20542E-15	***	***	***	***
1000	***	1.41614e-15	1.40284e-15	2.81898E-15	***	***	***	***
1200	***	5.87831e-15	5.21647e-15	1.10948E-14	***	***	***	***
1400	***	1.76015e-14	1.45825e-14	3.2184E-14	***	***	***	***
1600	***	4.23665e-14	3.34885e-14	7.5855E-14	***	***	***	***
1800	***	8.73309e-14	6.67029e-14	1.54034E-13	***	***	***	***
2000	***	1.60466e-13	1.19392e-13	2.79858E-13	***	***	***	***

10 atm

T (K)	R->W	R->Pa	R->Pb	R->	W->R	W->P1	W->P2	W->
100	2.20159E-10	5.89794e-38	1.15096e-22	2.20159E-10	1.7005E-10	9.39971e-46	7.01178e-21	1.7005E-10
120	2.30573E-10	4.49562e-34	2.79952e-22	2.30573E-10	3.46562E-6	3.60733e-37	8.02267e-17	3.46562E-6
140	2.28983E-10	2.74484e-31	5.95499e-22	2.28983E-10	0.0039	7.0098e-32	6.74486e-14	0.0039
160	2.17658E-10	3.46324e-29	1.14218e-21	2.17658E-10	0.70867	8.95366e-28	1.07672e-11	0.70867
180	1.99573E-10	1.52825e-27	2.03055e-21	1.99573E-10	38.0053	3.9542e-24	5.54787e-10	38.0053
200	1.77734E-10	3.23244e-26	3.43004e-21	1.77734E-10	863.977	2.72481e-21	1.27513e-08	863.977
220	1.54634E-10	4.00369e-25	5.62058e-21	1.54634E-10	10503.89	5.81059e-19	1.61359e-07	10503.89
240	1.32028E-10	3.31844e-24	9.08117e-21	1.32028E-10	79793.9	5.09224e-17	1.29753e-06	79793.9
260	1.11016E-10	2.01851e-23	1.46359e-20	1.11016E-10	422011	2.23243e-15	7.33699e-06	422011.0
280	9.21797E-11	9.62411e-23	2.36898e-20	9.21797E-11	1.67898E6	5.70203e-14	3.13948e-05	1.67898E6
298	7.73045E-11	3.3181e-22	3.67446e-20	7.73045E-11	4.78458E6	7.22457e-13	9.58361e-05	4.78458E6
350	4.48515E-11	6.08516e-21	1.32449e-19	4.48515E-11	4.55582E7	2.47361e-10	0.00112527	4.55582E7
400	2.58601E-11	5.17089e-20	4.38541e-19	2.58601E-11	1.90118E8	1.56083e-08	0.00580428	1.90118E8
500	8.74428E-12	1.16401e-18	3.62105e-18	8.74428E-12	1.04846E9	5.10624e-06	0.0502442	1.04846E9
600	***	1.04194e-17	1.98472e-17	3.02666E-17	***	***	***	***
700	***	5.43262e-17	7.83505e-17	1.32677E-16	***	***	***	***
800	***	2.00096e-16	2.42389e-16	4.42485E-16	***	***	***	***
900	***	5.80355e-16	6.25061e-16	1.20542E-15	***	***	***	***
1000	***	1.41614e-15	1.40284e-15	2.81898E-15	***	***	***	***

1200	***	5.87831e-15	5.21647e-15	1.10948E-14	***	***	***	***
1400	***	1.76015e-14	1.45825e-14	3.2184E-14	***	***	***	***
1600	***	4.23665e-14	3.34885e-14	7.5855E-14	***	***	***	***
1800	***	8.73309e-14	6.67029e-14	1.54034E-13	***	***	***	***
2000	***	1.60466e-13	1.19392e-13	2.79858E-13	***	***	***	***

100 atm

T (K)	R->W	R->Pa	R->Pb	R->	W->R	W->P1	W->P2	W->
100	2.28534E-10	5.85845e-38	1.35057e-23	2.28534E-10	1.76518E-10	3.05037e-40	7.09024e-21	1.76518E-10
120	2.48575E-10	4.47379e-34	3.84942e-23	2.48575E-10	3.73619E-6	3.28145e-32	8.3856e-17	3.73619E-6
140	2.60553E-10	2.73517e-31	1.01133e-22	2.60553E-10	0.00443	1.64511e-26	7.58617e-14	0.00443
160	2.65407E-10	3.45437e-29	2.47926e-22	2.65407E-10	0.86413	2.88745e-22	1.36787e-11	0.86413
180	2.6414E-10	1.52537e-27	5.70283e-22	2.6414E-10	50.3009	5.47331e-19	8.32866e-10	50.3009
200	2.57837E-10	3.22792e-26	1.23733e-21	2.57837E-10	1253.343	2.19698e-16	2.34099e-08	1253.343
220	2.4752E-10	3.99947e-25	2.54785e-21	2.4752E-10	16812.76	2.86177e-14	3.70066e-07	16812.76
240	2.34111E-10	3.31577e-24	5.01513e-21	2.34111E-10	141476.6	1.60902e-12	3.75457e-06	141476.6
260	2.18398E-10	2.01726e-23	9.50963e-21	2.18398E-10	830034	4.73591e-11	2.6818e-05	830034.00
280	2.01142E-10	9.6195e-23	1.7487e-20	2.01142E-10	3.66204E6	8.39558e-10	0.00014431	3.66204E6
298	1.8487E-10	3.31683e-22	2.96001e-20	1.8487E-10	1.14326E7	7.88436e-09	0.000537584	1.14326E7
350	1.37799E-10	6.08389e-21	1.23016e-19	1.37799E-10	1.39418E8	1.27854e-06	0.0106645	1.39418E8
400	9.81731E-11	5.17028e-20	4.27768e-19	9.81731E-11	7.11621E8	4.43236e-05	0.0838112	7.11621E8
500	4.62942E-11	1.16396e-18	3.60958e-18	4.62942E-11	5.12648E9	0.0054466	1.31689	5.12648E9
600	***	1.04194e-17	1.98472e-17	3.02666E-17	***	***	***	***
700	***	5.43262e-17	7.83505e-17	1.32677E-16	***	***	***	***
800	***	2.00096e-16	2.42389e-16	4.42485E-16	***	***	***	***
900	***	5.80355e-16	6.25061e-16	1.20542E-15	***	***	***	***
1000	***	1.41614e-15	1.40284e-15	2.81898E-15	***	***	***	***
1200	***	5.87831e-15	5.21647e-15	1.10948E-14	***	***	***	***
1400	***	1.76015e-14	1.45825e-14	3.2184E-14	***	***	***	***
1600	***	4.23665e-14	3.34885e-14	7.5855E-14	***	***	***	***
1800	***	8.73309e-14	6.6703e-14	1.54034E-13	***	***	***	***
2000	***	1.60466e-13	1.19392e-13	2.79858E-13	***	***	***	***

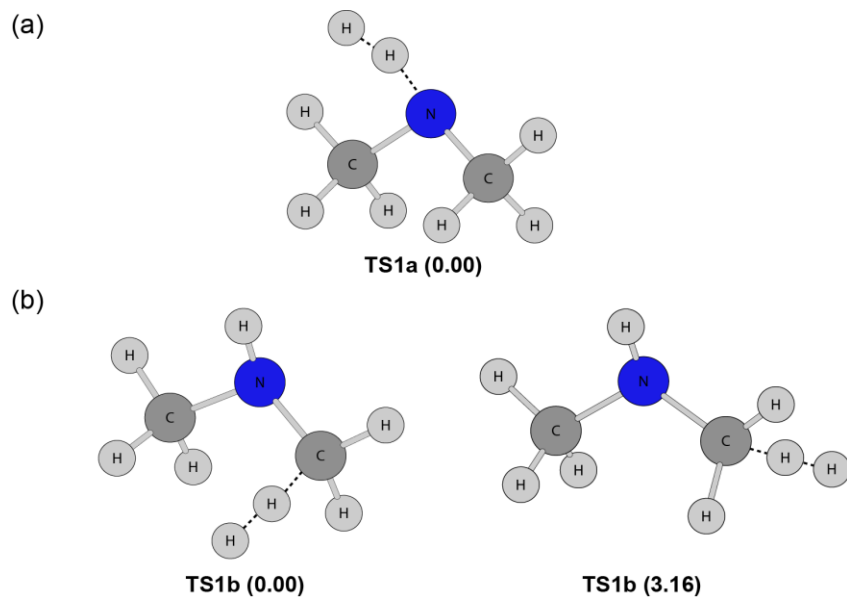


Figure S1: All distinguishable conformers for (a) TS1a and (b) TS1b. The values in parentheses are energies relative to the conformer with the lowest energy in kcal mol⁻¹.

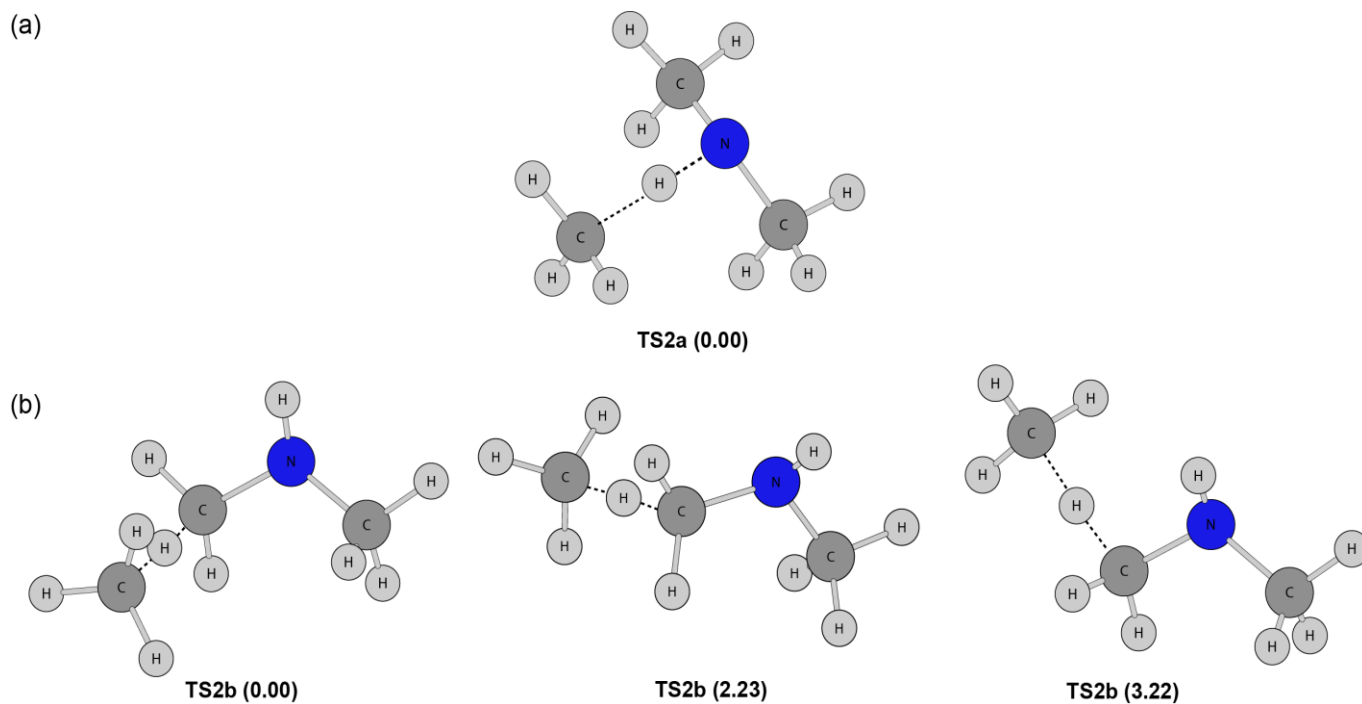
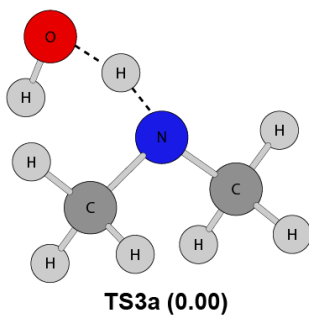


Figure S2: All distinguishable conformers for (a) TS2a and (b) TS2b. The values in parentheses are energies relative to the conformer with the lowest energy in kcal mol⁻¹.

(a)



(b)

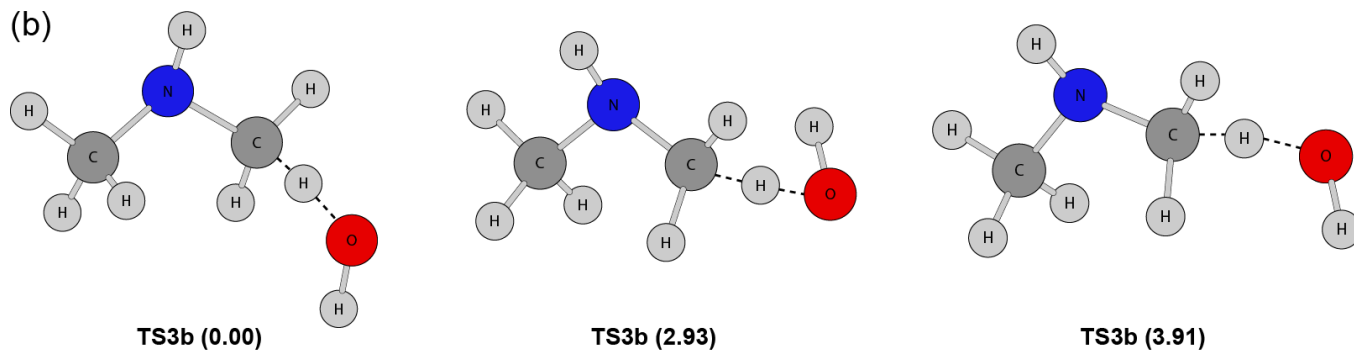
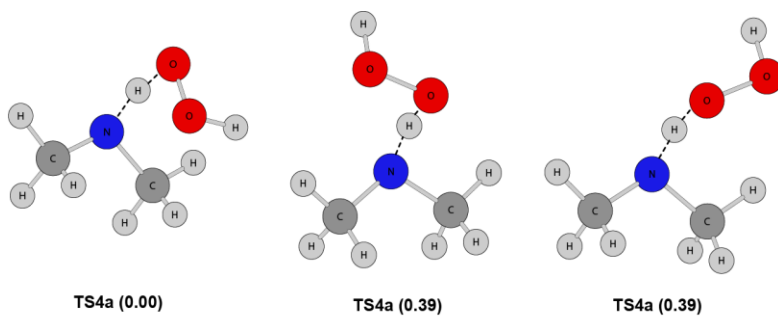


Figure S3: All distinguishable conformers for (a) TS3a and (b) TS3b. The values in parentheses are energies relative to the conformer with the lowest energy in kcal mol⁻¹.

(a)



(b)

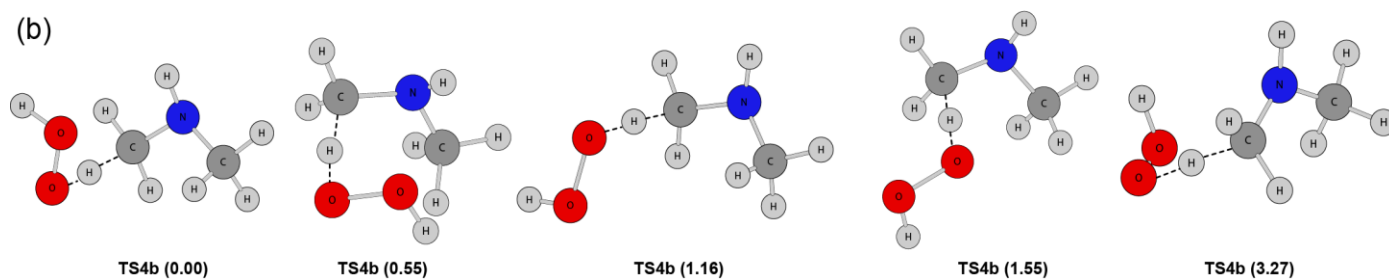


Figure S4: All distinguishable conformers for (a) TS4a and (b) TS4b. The values in parentheses are energies relative to the conformer with the lowest energy in kcal mol⁻¹.

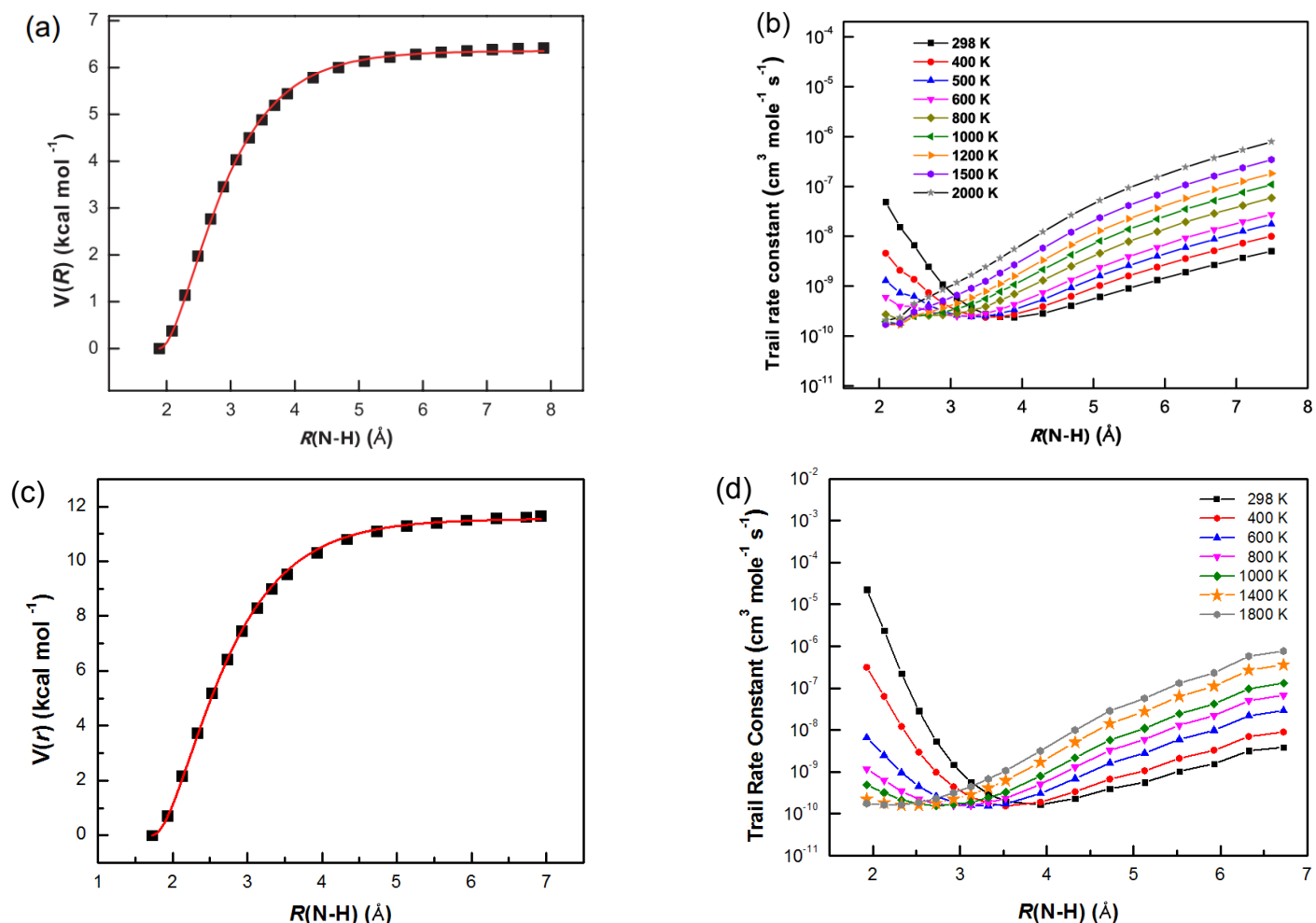


Figure S5: (a)(c) Relaxed scanning calculated at the CCSD(T)/CBS(D-T-Q)//BHandHLYP/cc-pVTZ level of the relative energy (including ZPE), and (b)(d) the calculated the “trail” rate constants at the different temperatures as the function of N-H bond length for entrance channel for DMA + OH/HO₂ reaction systems.

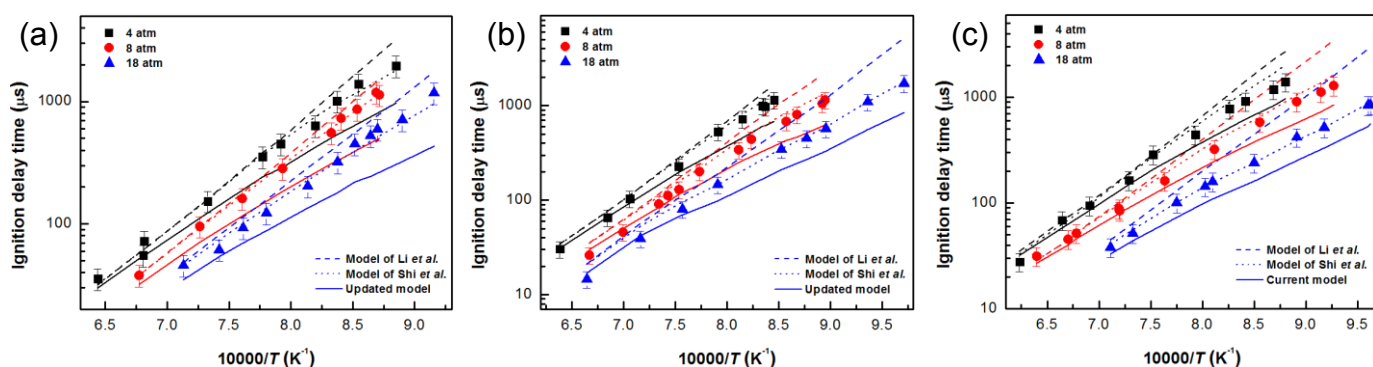
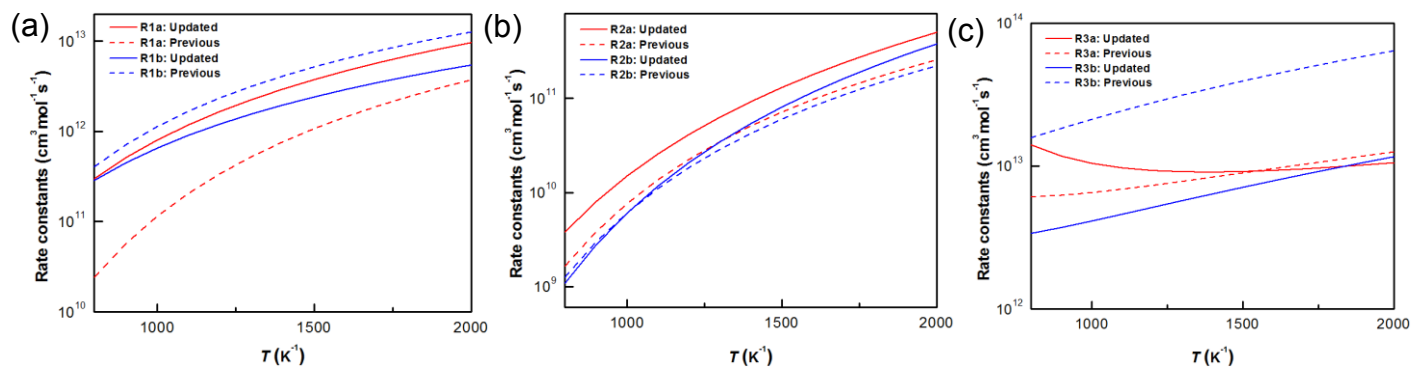


Figure S6: The comparisons between the prediction of the models from Li *et al.* (red dash line), Shi *et al.* (blue dot line), and this work (black solid line), and the experimental ignition delay times for DMA at pressure of 4, 8, 18 atm and equivalence ratio of (a) 0.5, (b) 1.0, and (c) 2.0.



The kinetic mechanism for bimolecular reaction

Figure S8: The kinetic mechanism for bimolecular reaction with the formation of reactant-complex (RC).

$$k_{\text{H}}(T) = k_{1,\infty}(T) \int_0^\infty \frac{k_2(E)}{k_{-1}(E) + k_2(E) + k_c[M]} dE \quad (1)$$

where the $k_{1,\infty}$ is the high-pressure limit rate constant for forming the RC; $k_{-1}(E)$ is the rate constant for unimolecular decomposition from RC to reactants; $k_2(E)$ is the rate constant for unimolecular reaction from RC to products; k_c is the collisional rate constant for deactivation of RC; $[M]$ is the concentration of the collider gas. Hence, the overall rate constant k is equal to the sum of k_H and k_S :

$$k = k_H + k_S = k_{1,\infty}(T) \int_0^\infty \frac{k_2(E) + k_c[M]}{k_{-1}(E) + k_2(E) + k_c[M]} \quad (3)$$

$$k^{\text{LPL}} = k_{1,\infty}(T) \int_0^\infty \frac{k_2(E)}{k_{-1}(E) + k_2(E)} = k_{1,\infty} \frac{k_2}{k_{-1} + k_2} \quad (4)$$

$$k^{\text{PEM}} = \frac{k_{1,\infty}}{k_{-1}} k_2 = K_{eq} k_2$$

$$k^{\text{HPL}} = k_{1,\infty}$$

An example of input file for ktools code in MultiWell program

Reactant complex => DMA + OH

KCAL MCC

both backup

70000 10.

500 1 ! Max J value to calculate sums and densities of state; step size of J

400 900 100000

20

100 200 298. 400. 500. 600. 700. 800. 900. 1000. 1100. 1200. 1300. 1400. 1500. 1600. 1700. 1800. 1900. 2000.

1 19 2

reac RC3-bh 0.000000 1.8860158935

C2H8NO

! Calculated at BHandHLYP/cc-pVTZ level

!

!

1 1 1

0.0 2

32 'HAR' AMUA

1	vib	51.3256	0.0	1
2	vib	76.3222	0.0	1
3	vib	193.6686	0.0	1
4	vib	224.3438	0.0	1
5	vib	284.9885	0.0	1
6	vib	402.7662	0.0	1
7	vib	630.8289	0.0	1
8	vib	782.7158	0.0	1
9	vib	885.5817	0.0	1
10	vib	972.1496	0.0	1
11	vib	1076.2168	0.0	1
12	vib	1141.3743	0.0	1
13	vib	1216.0452	0.0	1
14	vib	1252.9017	0.0	1
15	vib	1318.3611	0.0	1
16	vib	1501.9018	0.0	1
17	vib	1528.6239	0.0	1
18	vib	1532.8821	0.0	1
19	vib	1552.5950	0.0	1
20	vib	1554.6140	0.0	1
21	vib	1571.1814	0.0	1
22	vib	1573.1200	0.0	1
23	vib	3060.2227	0.0	1
24	vib	3062.9811	0.0	1
25	vib	3150.5924	0.0	1
26	vib	3152.9222	0.0	1
27	vib	3192.5012	0.0	1
28	vib	3192.7237	0.0	1
29	vib	3497.1900	0.0	1
30	vib	3646.0912	0.0	1

31	kro	58.6281	1.0	1	! K-rotor
32	jro	157.7471	1.0	2	! 2D adiabatic rotor

ctst RC3Morse-1 0.376786287148693 2.0860158935

C2H8NO

! Calculated at BHandHLYP/cc-pVTZ level

! Stepsize = 0.2 A

! Trail

1 1 1

0.0 2

31 'HAR' AMUA

1	vib	53.6325	0.0	1	
2	vib	55.0295	0.0	1	
3	vib	227.2063	0.0	1	
4	vib	258.7020	0.0	1	
5	vib	390.6652	0.0	1	
6	vib	537.7518	0.0	1	
7	vib	605.0747	0.0	1	
8	vib	801.4280	0.0	1	
9	vib	962.9757	0.0	1	
10	vib	1074.8000	0.0	1	
11	vib	1141.6560	0.0	1	
12	vib	1147.2592	0.0	1	
13	vib	1216.7827	0.0	1	
14	vib	1318.1466	0.0	1	
15	vib	1476.6405	0.0	1	
16	vib	1500.5805	0.0	1	
17	vib	1528.2139	0.0	1	
18	vib	1532.5963	0.0	1	
19	vib	1547.0135	0.0	1	
20	vib	1562.4379	0.0	1	
21	vib	1572.5369	0.0	1	
22	vib	1572.9416	0.0	1	
23	vib	3053.5196	0.0	1	
24	vib	3056.5853	0.0	1	
25	vib	3147.3770	0.0	1	
26	vib	3148.3826	0.0	1	
27	vib	3188.4936	0.0	1	
28	vib	3188.8964	0.0	1	
29	vib	3651.5564	0.0	1	
30	kro	58.8497	1.0	1	! K-rotor
31	jro	171.2100	1.0	2	! 2D adiabatic rotor

ctst RC3Morse-2 1.13665908835849 2.2860158935

C2H8NO

! Calculated at BHandHLYP/cc-pVTZ level

! Stepsize = 0.2 A

! Trail

1 1 1

0.0		2		
31 'HAR'	AMUA			
1	vib	47.7321	0.0	1
2	vib	64.2314	0.0	1
3	vib	232.2056	0.0	1
4	vib	260.3403	0.0	1
5	vib	391.1340	0.0	1
6	vib	444.3664	0.0	1
7	vib	526.8556	0.0	1
8	vib	782.4079	0.0	1
9	vib	963.8020	0.0	1
10	vib	1075.2135	0.0	1
11	vib	1142.2221	0.0	1
12	vib	1149.4760	0.0	1
13	vib	1218.6937	0.0	1
14	vib	1318.2103	0.0	1
15	vib	1458.5909	0.0	1
16	vib	1500.8796	0.0	1
17	vib	1532.1676	0.0	1
18	vib	1533.0919	0.0	1
19	vib	1550.5737	0.0	1
20	vib	1555.8129	0.0	1
21	vib	1573.6893	0.0	1
22	vib	1607.3096	0.0	1
23	vib	3048.3806	0.0	1
24	vib	3051.7165	0.0	1
25	vib	3145.0119	0.0	1
26	vib	3146.5195	0.0	1
27	vib	3187.2501	0.0	1
28	vib	3188.1718	0.0	1
29	vib	3651.5603	0.0	1
30	kro	58.5793	1.0	1 ! K-rotor
31	jro	189.5898	1.0	2 ! 2D adiabatic rotor

...
...

ctst RC3Morse-17 6.35802866876908 6.6860158935
C2H8NO

! Calculated at BHandHLYP/cc-pVTZ level

! Stepsize = 0.2 A

! Trai

1 1 1

0.0		2		
31 'HAR'	AMUA			
1	vib	8.1968	0.0	1
2	vib	14.8986	0.0	1
3	vib	57.6628	0.0	1
4	vib	60.6361	0.0	1
5	vib	231.3190	0.0	1
6	vib	258.6501	0.0	1

7	vib	382.1212	0.0	1	
8	vib	715.7767	0.0	1	
9	vib	953.4115	0.0	1	
10	vib	1073.8307	0.0	1	
11	vib	1143.6169	0.0	1	
12	vib	1147.5587	0.0	1	
13	vib	1225.7156	0.0	1	
14	vib	1317.0446	0.0	1	
15	vib	1481.0063	0.0	1	
16	vib	1497.4197	0.0	1	
17	vib	1532.3301	0.0	1	
18	vib	1534.3444	0.0	1	
19	vib	1542.5730	0.0	1	
20	vib	1559.4650	0.0	1	
21	vib	1574.0614	0.0	1	
22	vib	1581.3238	0.0	1	
23	vib	3023.7248	0.0	1	
24	vib	3028.1361	0.0	1	
25	vib	3131.1702	0.0	1	
26	vib	3131.7397	0.0	1	
27	vib	3176.4135	0.0	1	
28	vib	3177.6034	0.0	1	
29	vib	3655.4423	0.0	1	
30	kro	58.6170	1.0	1	! K-rotor
31	jro	813.1684	1.0	2	! 2D adiabatic rotor

ctst RC3Morse-18 6.3836906673501 7.0860158935

C2H8NO

! Calculated at BHandHLYP/cc-pVTZ level

! Stepsize = 0.2 A

! Trai

1 1 1

0.0 2

31 'HAR' AMUA

1	vib	7.7805	0.0	1
2	vib	13.8719	0.0	1
3	vib	53.3276	0.0	1
4	vib	54.7660	0.0	1
5	vib	231.3142	0.0	1
6	vib	258.4404	0.0	1
7	vib	381.9368	0.0	1
8	vib	714.7358	0.0	1
9	vib	953.5041	0.0	1
10	vib	1073.8572	0.0	1
11	vib	1143.8600	0.0	1
12	vib	1148.8047	0.0	1
13	vib	1225.8496	0.0	1
14	vib	1317.1900	0.0	1
15	vib	1490.2239	0.0	1

16	vib	1498.0686	0.0	1	
17	vib	1532.9839	0.0	1	
18	vib	1535.1204	0.0	1	
19	vib	1542.6190	0.0	1	
20	vib	1559.9575	0.0	1	
21	vib	1574.0776	0.0	1	
22	vib	1585.4127	0.0	1	
23	vib	3023.4409	0.0	1	
24	vib	3027.8183	0.0	1	
25	vib	3131.1264	0.0	1	
26	vib	3131.7460	0.0	1	
27	vib	3176.3976	0.0	1	
28	vib	3177.5469	0.0	1	
29	vib	3655.5728	0.0	1	
30	kro	58.6563	1.0	1	! K-rotor
31	jro	893.1054	1.0	2	! 2D adiabatic rotor

ctst RC3Morse-19 6.40389103115895 7.4860158935

C2H8NO

! Calculated at BHandHLYP/cc-pVTZ level

! Stepsize = 0.2 A

! Trai

1 1 1

0.0 2

31 'HAR' AMUA

1	vib	7.4118	0.0	1
2	vib	12.9535	0.0	1
3	vib	49.4423	0.0	1
4	vib	49.5689	0.0	1
5	vib	231.3111	0.0	1
6	vib	258.2004	0.0	1
7	vib	381.7036	0.0	1
8	vib	709.2664	0.0	1
9	vib	952.7268	0.0	1
10	vib	1073.8778	0.0	1
11	vib	1143.7964	0.0	1
12	vib	1151.7386	0.0	1
13	vib	1225.9701	0.0	1
14	vib	1316.9864	0.0	1
15	vib	1486.3696	0.0	1
16	vib	1497.3974	0.0	1
17	vib	1531.5701	0.0	1
18	vib	1533.9736	0.0	1
19	vib	1542.9773	0.0	1
20	vib	1556.6171	0.0	1
21	vib	1573.7142	0.0	1
22	vib	1577.4062	0.0	1
23	vib	3023.1821	0.0	1
24	vib	3027.7233	0.0	1

25	vib	3131.0877	0.0	1	
26	vib	3131.8666	0.0	1	
27	vib	3176.3850	0.0	1	
28	vib	3177.5792	0.0	1	
29	vib	3655.7365	0.0	1	
30	kro	58.6912	1.0	1	! K-rotor
31	jro	976.9990	1.0	2	! 2D adiabatic rotor

prod OH 3.21 10.
HO

! Calculated at BHandHLYP/cc-pVTZ level

!

!

1 1 5

0.0 2

139.05 2

32403. 2

68372. 2

89420. 2

2 'HAR' AMUA

1	vib	3868.7879	0.0	1	
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2	jro	0.8777	1.0	2	! 2D adiabatic rotor
---	-----	--------	-----	---	----------------------

prod DMA 3.21 10.

C2H7N

! Calculated at BHandHLYP/cc-pVTZ level

!

!

1 1 1

0.0 1

26 'HAR' AMUA

1	vib	230.9903	0.0	1	
---	-----	----------	-----	---	--

2	vib	266.4736	0.0	1	
---	-----	----------	-----	---	--

3	vib	393.8462	0.0	1	
---	-----	----------	-----	---	--

4	vib	795.7013	0.0	1	
---	-----	----------	-----	---	--

5	vib	978.8876	0.0	1	
---	-----	----------	-----	---	--

6	vib	1074.1769	0.0	1	
---	-----	-----------	-----	---	--

7	vib	1143.9036	0.0	1	
---	-----	-----------	-----	---	--

8	vib	1226.5776	0.0	1	
---	-----	-----------	-----	---	--

9	vib	1235.9092	0.0	1	
---	-----	-----------	-----	---	--

10	vib	1317.8331	0.0	1	
----	-----	-----------	-----	---	--

11	vib	1496.9604	0.0	1	
----	-----	-----------	-----	---	--

12	vib	1525.5063	0.0	1	
----	-----	-----------	-----	---	--

13	vib	1532.9725	0.0	1	
----	-----	-----------	-----	---	--

14	vib	1542.8525	0.0	1	
----	-----	-----------	-----	---	--

15	vib	1550.0842	0.0	1	
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16	vib	1571.1400	0.0	1	
----	-----	-----------	-----	---	--

17	vib	1574.5726	0.0	1	
----	-----	-----------	-----	---	--

18	vib	3021.6735	0.0	1	
----	-----	-----------	-----	---	--

19	vib	3026.0300	0.0	1	
20	vib	3131.1304	0.0	1	
21	vib	3131.6048	0.0	1	
22	vib	3176.5074	0.0	1	
23	vib	3177.3093	0.0	1	
24	vib	3657.1043	0.0	1	
25	kro	14.2467	1.0	1	! K-rotor
26	jro	56.9856	1.0	2	! 2D adiabatic rotor

An example of input file for multiwell code in MultiWell program

DMA+OH => DMA~OH(RC3) => TS3a => Products

10. 400 900 100000 2113989025

'ATM' 'KCAL' 'AMUA'

1300 1300

3

0.001 1.2 100

1 2

1 'ktools-rc' -6.42 157.7471 1 2 1

2 'Reactant' 0.00

3 'Channel-a' -25.08

3.32 144 40 62 !Ar

1 5.40 307 1 200. 0 0. 0. 0. 0. 0. 0.

'LJ'

2

1 2 'ktools-ts' 189.5898 1 2 1 1E+16 6.42 REV FAST NOTUN CENT2 SUM

1 3 'TS3a' 121.4706 1 2 1 3E+13 1.42 REV FAST TUN NOCENT SUM

TUN 1045.3728

1E+7 COLL 1000 CHEMACT 1 3 0