

An Experimental and Theoretical Study of the High Temperature Reactions of Four Butyl Radical Isomers

John B. Randazzo, Ahren W. Jasper, Raghu Sivaramakrishnan, Travis Sikes, Patrick T. Lynch, and Robert S. Tranter

Phys. Chem. Chem. Phys.

***iso*-Pentyl nitrite**

Table S1. List of experimental conditions and rate coefficients for $k_{1,1}$ ($i\text{-C}_5\text{H}_{11}\text{ONO} = i\text{-C}_5\text{H}_{11}\text{O} + \text{NO}$)

[$i\text{-C}_5\text{H}_{11}\text{ONO}$]	P_1 / Torr	T_1 / °C	P_2 / Torr	T_2 / K	$k_{1,1}/\text{s}^{-1}$
1%	8.0	24.5	62	787	2.353E+04
1%	7.5	24.5	63	825	6.553E+04
1%	7.0	24.5	66	890	1.971E+05
1%	6.5	24.5	65	926	5.040E+05
1%	6.0	24.5	63	958	9.521E+05
1%	18.5	24.5	127	726	5.614E+03
1%	17.5	24.5	130	764	1.852E+04
1%	16.5	24.0	133	805	5.795E+04
1%	15.5	24.0	132	833	1.367E+05
1%	14.5	24.2	130	864	2.893E+05
1%	13.5	24.2	130	903	5.066E+05
1%	29.0	24.0	231	797	6.679E+04
1%	32.0	24.0	265	818	1.047E+05
1%	29.0	24.0	245	829	1.562E+05
1%	29.0	24.0	283	913	7.262E+05
1%	27.0	24.0	278	946	1.083E+06
2%	8.0	23.9	62	735	6.165E+03
2%	7.5	23.9	64	778	2.317E+04
2%	7.0	23.9	64	814	7.112E+04

2%	7.0	23.8	69	853	2.534E+05
2%	6.0	23.8	64	899	5.505E+05
2%	5.5	23.9	64	949	1.074E+06
2%	18.0	22.6	128	696	2.495E+03
2%	18.0	23.3	129	701	2.344E+03
2%	18.0	23.0	130	706	3.180E+03
2%	17.0	23.0	130	729	6.065E+03
2%	17.0	23.3	130	729	5.526E+03
2%	17.0	22.6	131	730	6.582E+03
2%	16.0	23.3	129	753	1.342E+04
2%	16.0	23.0	131	757	1.293E+04
2%	16.0	22.6	134	767	2.330E+04
2%	15.0	22.6	130	786	4.462E+04
2%	15.0	23.3	131	789	3.929E+04
2%	15.0	23.0	131	791	5.300E+04
2%	14.0	23.0	132	823	1.477E+05
2%	14.0	23.3	131	826	1.643E+05
2%	14.0	22.6	136	843	2.511E+05
2%	14.5	22.6	142	849	3.019E+05
2%	13.0	22.6	130	861	3.599E+05
2%	14.5	23.0	147	867	4.317E+05
2%	13.0	23.3	133	873	4.081E+05
2%	13.0	23.0	135	879	5.966E+05
2%	12.0	22.6	128	897	7.852E+05
2%	12.0	23.3	129	901	8.488E+05

2%

12.0

23.0

132

914

2.495E+03

***sec*-Pentyl nitrite**

Table S2. List of experimental conditions and rate coefficients for k_{2.2} (2-C₅H₁₁ONO = 2-C₅H₁₁O + NO)

[2-C ₅ H ₁₁ ONO]	P ₁ / Torr	T ₁ / °C	P ₂ / Torr	T ₂ / K	k _{2.2} / s ⁻¹
0.5%	18.5	21.4	129	752	1.209E+04
0.5%	17.5	21.4	129	781	2.669E+04
0.5%	16.5	21.4	131	820	6.026E+04
0.5%	15.5	21.4	131	853	1.264E+05
0.5%	14.5	21.4	131	897	2.750E+05
0.5%	13.5	21.4	128	927	3.871E+05
0.5%	12.5	21.4	126	967	6.945E+05
0.5%	37.0	21.4	251	739	9.605E+03
0.5%	33.0	21.4	255	805	4.733E+04
0.5%	30.0	21.4	258	865	1.824E+05
0.0%	27.0	21.4	255	922	6.329E+05
1%	9.0	21.3	62	723	5.986E+03
1%	8.0	21.3	61	772	1.853E+04
1%	7.5	21.3	62	814	4.163E+04
1%	7.0	21.3	63	859	9.041E+04
1%	6.5	21.3	64	910	2.514E+05
1%	6.0	21.3	64	966	5.432E+05
1%	18.5	21.3	128	725	5.554E+03
1%	17.5	21.3	130	756	1.220E+04
1%	16.5	21.3	132	793	3.565E+04
1%	15.5	21.3	133	829	7.523E+04
1%	14.5	21.3	131	861	1.689E+05

1%	13.5	21.3	132	906	3.708E+05
1%	12.5	21.3	130	945	7.519E+05
1%	37.0	21.3	251	716	4.264E+03
1%	33.0	21.3	255	776	2.946E+04
1%	30.0	21.3	258	832	1.123E+05
1%	27.0	21.3	258	892	3.555E+05

***neo*-Pentyl nitrite**

Table S3. List of experimental conditions and rate coefficients for $k_{3,3}$ ($\text{neo-C}_5\text{H}_{11}\text{ONO} = \text{neo-C}_5\text{H}_{11}\text{O} + \text{NO}$)

[neo-C ₅ H ₁₁ ONO]	P ₁ / Torr	T ₁ / °C	P ₂ / Torr	T ₂ / K	k _{2,2} / s ⁻¹
1%	9.0	21.2	62	722	6.484E+03
1%	8.0	21.2	61	769	1.927E+04
1%	7.5	21.2	62	812	4.513E+04
1%	7.0	21.2	63	857	8.715E+04
1%	6.5	21.2	63	901	1.675E+05
1%	18.5	21.5	128	726	7.238E+03
1%	17.5	21.5	129	755	1.323E+04
1%	16.5	21.5	131	789	3.239E+04
1%	15.5	21.5	131	822	6.752E+04
1%	14.5	21.5	131	858	1.418E+05
1%	13.5	21.5	129	891	2.187E+05
1%	12.5	21.5	127	929	4.756E+05
1%	37.0	21.4	250	714	4.536E+03
1%	33.0	21.4	257	779	3.153E+04
1%	30.0	21.4	261	838	1.292E+05
1%	27.0	21.4	258	892	3.991E+05
2%	8.2	21.4	62	721	4.940E+03
2%	7.5	21.4	63	769	1.722E+04
2%	7.0	21.4	65	813	4.084E+04
2%	6.5	21.4	65	859	1.152E+05
2%	6.0	21.4	65	904	2.847E+05
2%	5.5	21.4	65	955	6.350E+05

2%	17.0	21.4	128	719	5.210E+03
2%	16.0	21.4	130	750	1.167E+04
2%	15.0	21.4	130	782	2.700E+04
2%	14.0	21.4	130	815	6.051E+04
2%	13.5	21.4	132	845	1.334E+05
2%	13.0	21.4	135	876	2.609E+05
2%	12.0	21.4	132	911	5.127E+05
2%	11.0	21.4	131	959	1.077E+06
0.5%	18.5	21.4	129	752	1.209E+04

***n*-Pentyl nitrite**

Table S4. List of experimental conditions and rate coefficients for $k_{3,3}$ ($\text{n-C}_5\text{H}_{11}\text{ONO} = \text{n-C}_5\text{H}_{11}\text{O} + \text{NO}$)

[n-C₅H₁₁ONO]	P₁ / Torr	T₁ / °C	P₂ / Torr	T₂ / K	k_{2,2}/ s⁻¹
1%	18.5	21.5	127	722	5.779E+03
1%	17.0	21.5	127	762	1.602E+04
1%	16.0	21.5	128	796	3.052E+04
1%	15.5	21.5	131	822	7.144E+04
1%	14.5	21.5	131	859	1.816E+05
1%	13.5	21.5	131	901	4.236E+05
1%	12.5	21.5	127	930	7.270E+05
1%	11.5	21.5	124	973	1.212E+06
1%	37.0	21.5	249	713	3.494E+03
1%	33.0	21.5	251	770	2.224E+04
1%	30.0	21.5	254	825	1.081E+05
1%	27.0	21.5	256	888	4.138E+05
2%	8.2	21.4	61	718	4.517E+03
2%	7.5	21.4	62	765	1.361E+04
2%	7.0	21.4	64	808	4.049E+04
2%	6.5	21.4	65	857	1.566E+05
2%	6.0	21.4	66	908	4.341E+05
2%	5.5	21.4	64	948	6.265E+05
2%	5.0	21.4	64	1007	1.644E+06
2%	17.0	21.4	127	717	3.955E+03
2%	16.0	21.4	129	749	1.001E+04
2%	15.0	21.4	130	785	2.947E+04

2%	14.0	21.4	130	817	7.984E+04
2%	13.5	21.4	132	846	1.534E+05
2%	13.0	21.4	134	874	3.488E+05
1%	9.0	21.2	62	722	6.484E+03