

"Modeling the Organic Nitrate Yields in the Reaction of Alkyl Peroxy Radicals with Nitric Oxide. II. Reaction Simulations"

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Table S1. Vibrational Frequencies and Moments of Inertia for R = CH₃.¹

	RONO₂	ROONO	RO₂•	RO•
I _K / amu Å ²	42.8	23.56	8.398	3.213
I _{2D} / amu Å ²	127	185.1	46.66	18.13
Frequencies (cm ⁻¹)	131.0 (16.99,2) ^a	62.5 (21.46,1) ^a	134 (2.937,3) ^a	683.2
	193.2 (3.144,3) ^a	187 (3.189,3) ^a	490.1	957.3
	335.4	284 (19.19,1) ^a	909.2	1103.2
	569.3	320.1	1123.5	1353.3
	661.8	428.7	1147.8	1364.6
	768.7	511.6	1214.5	1510.2
	863.4	781.6	1442.0	2889.6
	1013.9	929.5	1468.8	2964.4
	1163.5	998.0	1480.4	3007.5
	1188.1	1164.9	3048.4	
	1323.4	1205.2	3139.3	
	1458.3	1449.1	3156.2	
	1469.5	1464.2		
	1498.0	1503.4		
	1713.0	1792.9		
	3052.1	3025.9		
	3135.5	3103.1		
	3155.8	3126.9		

^a Hindered internal rotation (I_r, n_r given in parentheses)

Table S2. Vibrational Frequencies and Moments of Inertia for R = i-C₃H₇.¹

	RONO₂	ROONO	RO₂•	RO•
I _K / amu Å ²	98.6	99.0	76.0	105
I _{2D} / amu Å ²	308	333	128	58.8
Frequencies (cm ⁻¹)	29.8	48.6	116.3	186.6
	47.2	75.6	206.6	229.4
	206.3	205.6	206.6	359.1
	212.0	217.4	297.4	391.7
	260.2	240.7	372.8	450.2
	322.3	284.6	388.2	802.5
	406.9	358.3	605.4	881.4
	452.5	378.2	755.6	913.4
	562.6	445.6	896.2	973.8
	562.6	485.1	938.6	1042.7
	768.1	519.7	945.4	1058.1
	856.9	798.4	1110.5	1150.7
	876.0	845.9	1144.2	1196.4
	916.4	902.0	1158.4	1244.9
	942.9	932.8	1206.1	1383.4
	952.3	940.2	1358.6	1407.4
	1129.1	953.5	1373.8	1478.0
	1160.8	1130.9	1399.7	1483.3
	1201.2	1165.7	1414.1	1493.7
	1313.4	1197.1	1477.9	1501.5
	1358.7	1355.3	1489.2	2821.5
	1388.2	1371.1	1493.7	3026.9
	1407.6	1405.0	1511.0	3034.0
	1423.4	1419.0	3037.7	3093.7
	1481.5	1479.6	3041.4	3099.9
	1485.7	1488.0	3069.7	3114.0
	1498.0	1493.9	3104.9	3115.3
	1511.6	1512.1	3108.4	
	1698.2	1780.5	3116.8	
	3036.8	3029.3	3122.7	
	3041.3	3033.4	127.63	
	3082.7	3039.5	76.027	
	3101.6	3097.9		
	3111.8	3108.0		
	3118.2	3116.4		
	3122.7	3117.7		

Table S3. Vibrational Frequencies and Moments of Inertia for R = 2-C₅H₁₁¹ and NO_x.

	RONO₂	ROONO	RO₂•	RO•	NO₂	NO
I _K / amu Å ²	193	238	119	63.9	2.086	---
I _{2D} / amu Å ²	637	603	371	314	39.8	9.84
Vibrations (cm ⁻¹)	61.6	46.4	76.4	96.0	1318.0	1876.1
	66.5	56.9	78.4	102.0	749.6	
	73.7	80.4	139.8	162.9	1617.8	
	116.0	104.1	172.9	221.2		
	178.6	175.9	215.8	241.6		
	213.6	216.3	242.5	316.6		
	239.9	226.5	295.7	362.4		
	243.8	238.7	316.7	409.3		
	296.0	272.4	396.4	481.5		
	350.0	305.9	467.6	747.6		
	463.8	385.7	600.1	843.4		
	480.4	409.1	747.6	856.7		
	564.6	456.8	765.4	894.3		
	700.6	488.6	876.1	905.3		
	751.4	552.1	882.8	971.6		
	767.8	737.4	933.0	1015.4		
	853.4	799.1	999.0	1047.0		
	870.4	847.0	1041.0	1065.7		
	882.1	874.9	1060.0	1115.7		
	901.6	888.2	1124.4	1146.5		
	942.3	925.4	1133.8	1248.8		
	1008.7	949.2	1156.8	1256.6		
	1042.1	1007.2	1192.2	1304.8		
	1062.3	1038.2	1269.6	1324.4		
	1134.8	1064.1	1299.7	1364.3		
	1146.5	1128.9	1333.7	1380.0		
	1191.6	1150.3	1364.3	1394.6		
	1270.0	1189.3	1380.3	1414.2		
	1295.0	1269.9	1402.2	1469.2		
	1316.5	1299.8	1408.2	1475.6		
	1332.8	1333.3	1416.3	1493.6		
	1362.1	1365.8	1474.7	1498.8		
	1390.1	1370.7	1487.3	1500.4		
	1404.6	1405.1	1495.2	1508.2		
	1414.3	1411.7	1500.1	2913.1		
	1416.5	1413.8	1501.7	3002.3		
	1477.1	1473.8	1509.7	3008.7		
	1490.5	1488.8	3011.5	3017.3		
	1495.8	1494.8	3018.4	3034.2		
	1500.7	1499.1	3021.6	3041.3		
	1502.4	1502.2	3040.0	3053.2		
	1510.4	1510.5	3047.8	3078.6		

1695.8	1775.6	3058.2	3084.5
3012.0	3009.3	3070.0	3118.8
3017.6	3014.3	3083.8	3131.2
3021.2	3018.4	3087.9	
3037.8	3021.7	3106.7	
3045.6	3036.3	3119.6	
3061.8	3045.7		
3080.0	3062.8		
3085.1	3084.3		
3089.3	3089.6		
3105.1	3101.1		
3118.9	3119.7		

References

- (1) Lohr, L. L.; Barker, J. R.; Shroll, R. M. *J. Phys. Chem. A.* **2003**, *in preparation*.