

## Electronic Supplementary Information

### Perdecanoic acid as a safe and stable medium-chain peracid for Baeyer-Villiger oxidation of cyclic ketones to lactones

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#### 1. Elemental analysis of peracids.

**Table S1.** Elemental analysis of peracids.

Peracid	Theoretical content of atoms, %			Determined content of atoms, <sup>a</sup> %		
	C	H	N	C	H	N
perC <sub>8</sub>	60.00	10.00	0.00	60.10	10.85	0.08
perC <sub>10</sub>	63.80	10.63	0.00	63.28	11.29	0.03
perC <sub>12</sub>	66.67	11.11	0.00	66.73	11.85	0.09

<sup>a</sup> average content based on three independent experiments

## 2. $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of peracids.

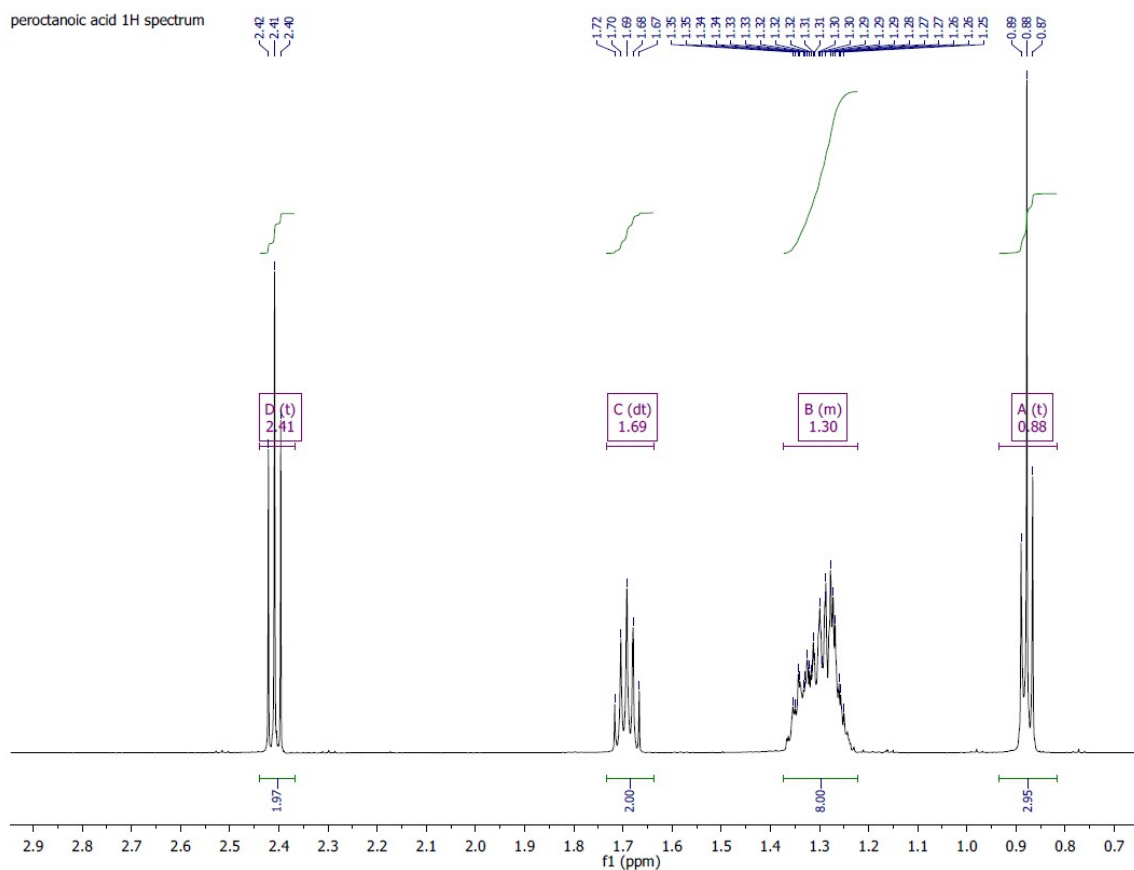


Figure S1.  $^1\text{H}$  NMR spectrum of peroctanoic acid.

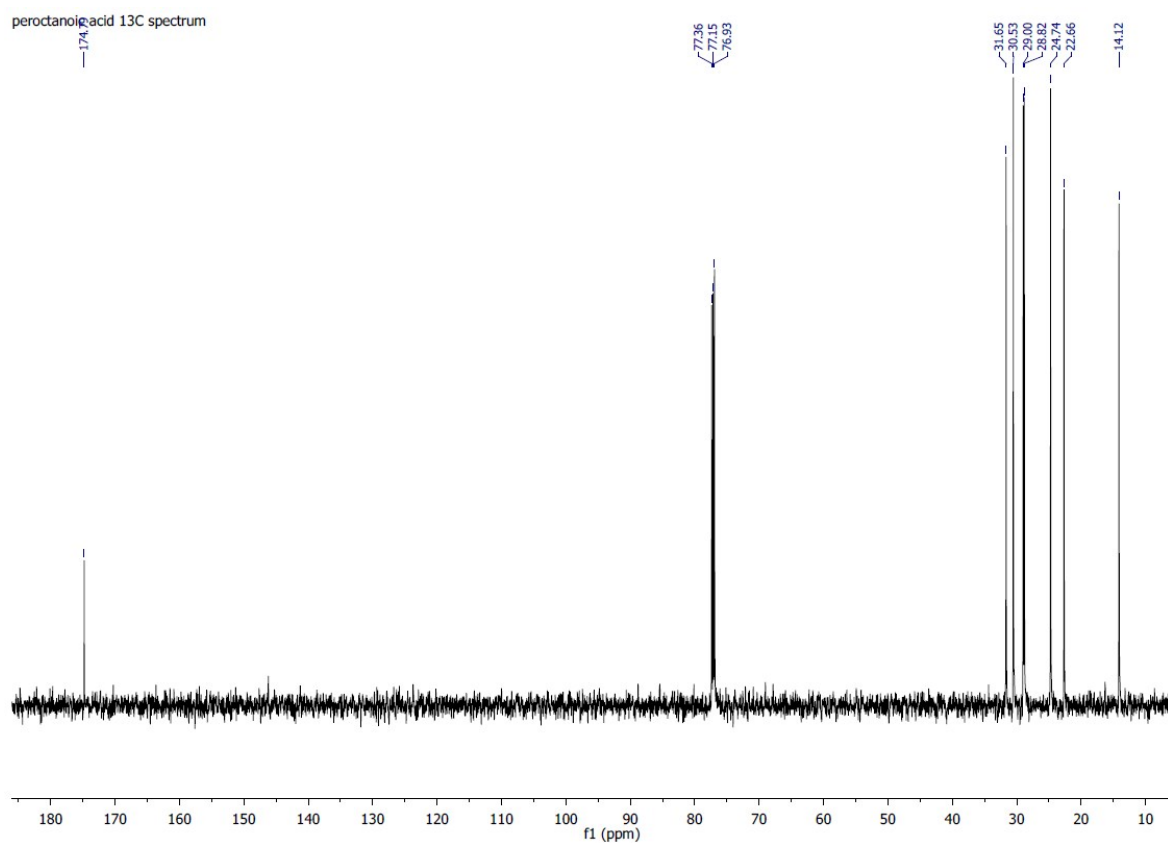


Figure S2.  $^{13}\text{C}$  NMR spectrum of peroctanoic acid.

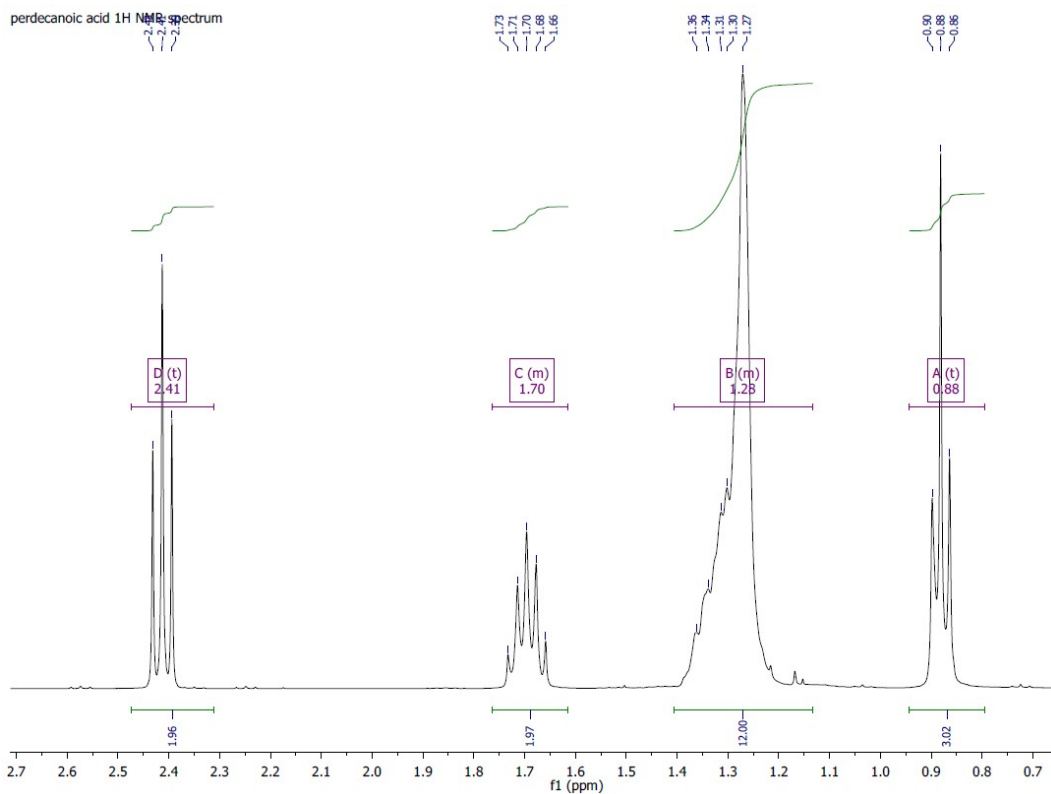


Figure S3. <sup>1</sup>H NMR spectrum of perdecanoic acid.

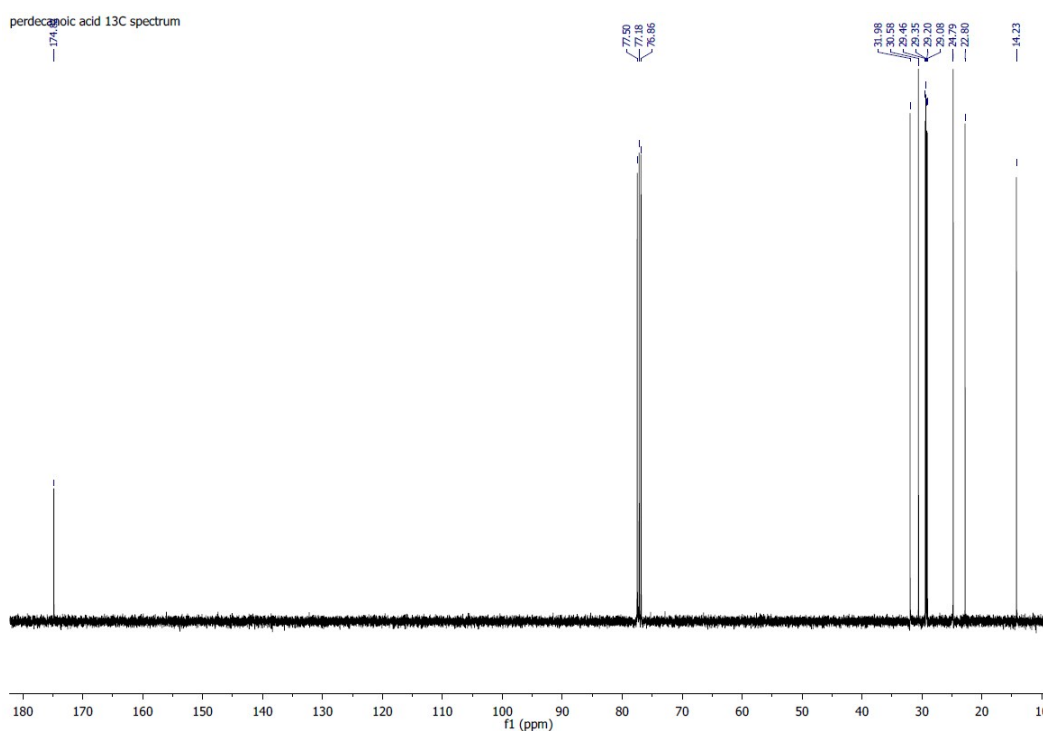


Figure S4. <sup>13</sup>C NMR spectrum of perdecanoic acid.

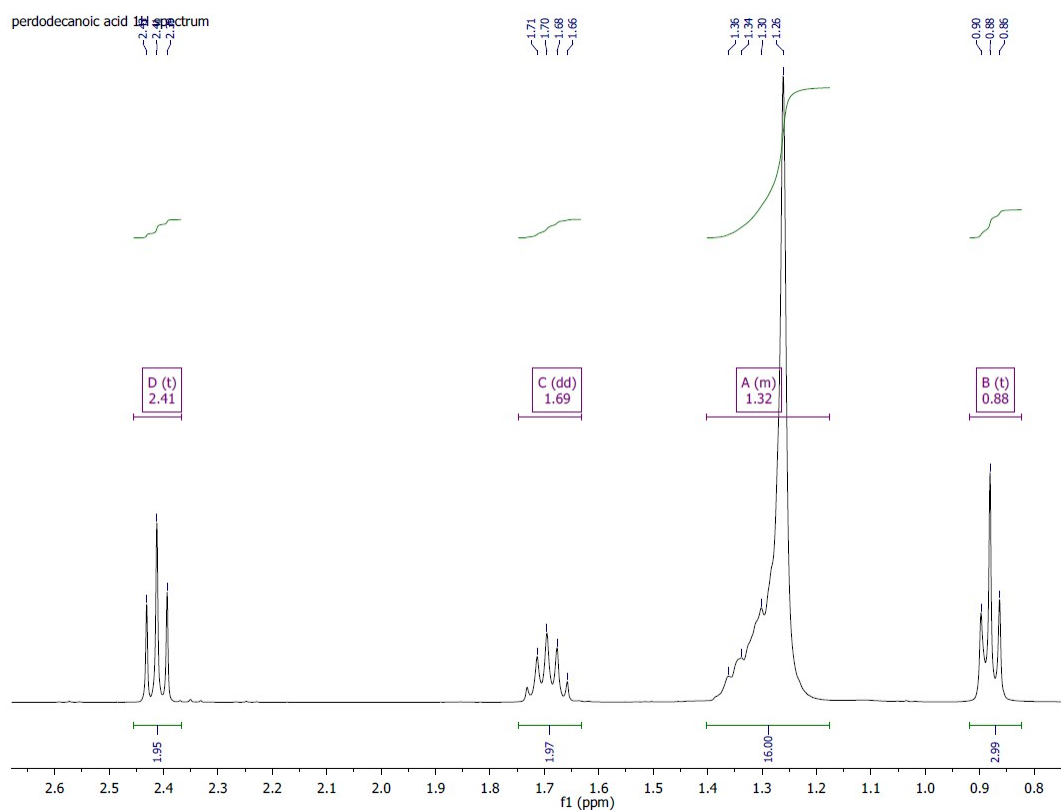


Figure S5. <sup>1</sup>H NMR spectrum of perdodecanoic acid.

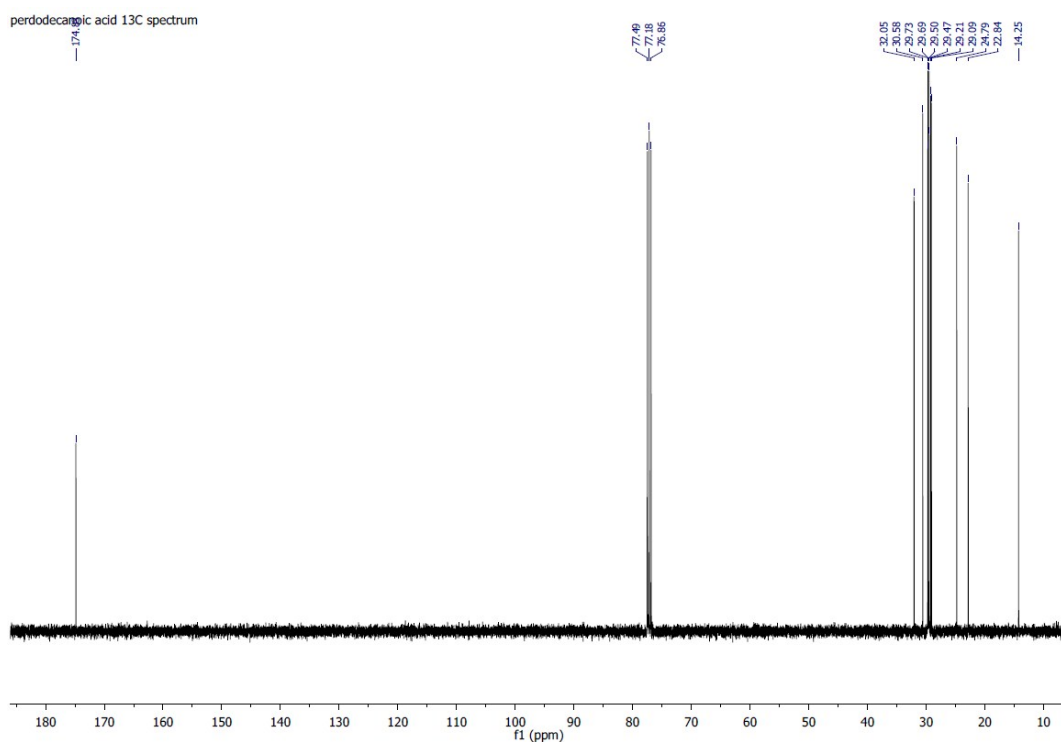
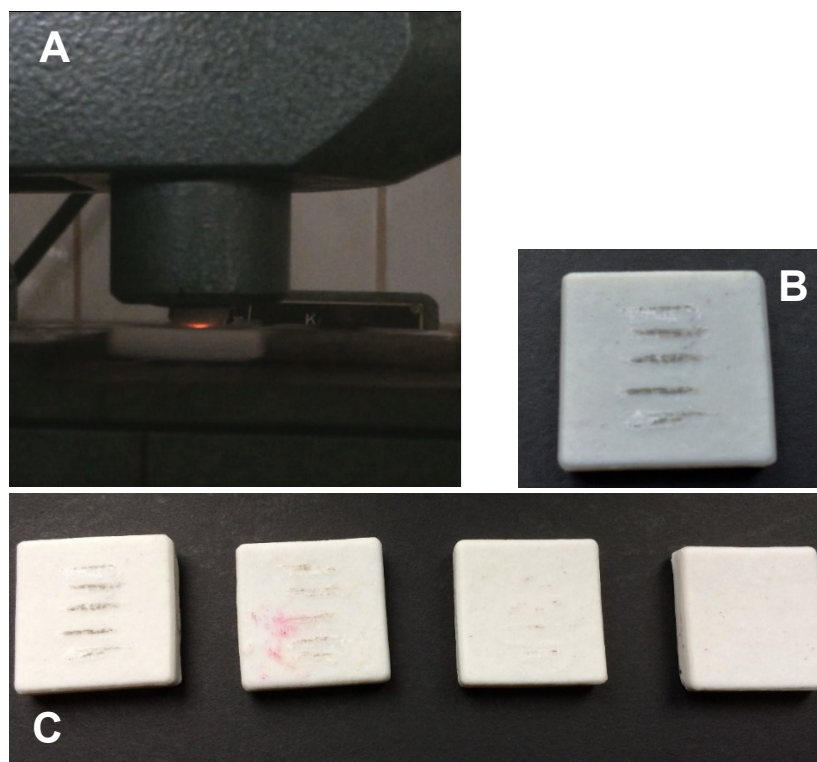


Figure S6. <sup>13</sup>C NMR spectrum of perdodecanoic acid.

### 3. Sensitivity of peracids to friction.



**Figure S7.** A: Positive effect of experiment – red flash; B: Positive effect of experiment – visible mark of decomposition on the plate; C: Comparison of plates showing the course of the experiments – from positive effect to negative effect/no effect (from left to right).

**Table S2.** Results for sensitivity to friction for perhexanoic acid; (+) positive effect of experiment, (-) negative effect of experiment.

Force / N	No. of experiment						Observed effect
	1	2	3	4	5	6	
353	+						red flash
157	+						visible mark of decomposition on the plate
118	+						visible mark of decomposition on the plate
110	+	+					visible mark of decomposition on the plate
106	+						visible mark of decomposition on the plate
96	+						visible mark of decomposition on the plate
82	+	+					visible mark of decomposition on the plate
78	-	+					visible mark of decomposition on the plate
71	+	+					visible mark of decomposition on the plate
63	-	+					visible mark of decomposition on the plate
59	+						visible mark of decomposition on the plate
55	+	-	+				visible mark of decomposition on the plate
53	+	+					visible mark of decomposition on the plate
47	-	-	+				visible mark of decomposition on the plate

Force / N	No. of experiment						Observed effect
	1	2	3	4	5	6	
41	-	-	-	-	-	-	no visible effect

**Table S3.** Results for sensitivity to friction for peroctanoic acid; (+) positive effect of experiment, (-) negative effect of experiment.

Force / N	No. of experiment						Observed effect
	1	2	3	4	5	6	
360	+						red flash
324	+						visible mark of decomposition on the plate
252	+						visible mark of decomposition on the plate
216	+						visible mark of decomposition on the plate
240	+						yellow flash
216	+	+					visible mark of decomposition on the plate
192	+						visible mark of decomposition on the plate
180	+	-	+	+			weakly visible mark of decomposition on the plate
168	+	+	+				yellow flash
160	+	+					visible mark of decomposition on the plate
144	+						visible mark of decomposition on the plate
128	+						visible mark of decomposition on the plate
112	+						weakly visible mark of decomposition on the plate
108	+						weakly visible mark of decomposition on the plate
96	+						weakly visible mark of decomposition on the plate
84	+						weakly visible mark of decomposition on the plate
80	+						weakly visible mark of decomposition on the plate
72	+	+					weakly visible mark of decomposition on the plate
64	-	+					weakly visible mark of decomposition on the plate

**Table S4.** Results for sensitivity to friction for perdecanoic acid; (+) positive effect of experiment, (-) negative effect of experiment.

Force / N	No. of experiment						Observed effect
	1	2	3	4	5	6	
353	+						visible mark of decomposition on the plate
157	+						visible mark of decomposition on the plate
141	+						visible mark of decomposition on the plate
125	-	-	-	-	+		visible mark of decomposition on the plate
118	-	+					visible mark of decomposition on the plate
110	+	-	+	-	+		visible mark of decomposition on the plate
106	-	-	-	-	-	-	no effect

**Table S5.** Results for sensitivity to friction for perdoecanoic acid; (+) positive effect of experiment, (-) negative effect of experiment.

Force / N	No. of experiment						Observed effect
	1	2	3	4	5	6	
353	+						visible mark of decomposition on the plate
157	+						visible mark of decomposition on the plate
125	+						visible mark of decomposition on the plate
118	+	-	-	-	+		visible mark of decomposition on the plate
110	-	-	-	-	-	-	no effect

#### 4. Sensitivity of peracids to shock.

**Table S6.** Results for sensitivity to shock for perhexanoic acid; (+) positive effect of experiment, (-) negative effect of experiment.

Weight / kg	Height / cm	Energy / J	No. of experiment						Observed effect
			1	2	3	4	5	6	
1	50	5	-						no effect
5	60	30	-						no effect
10	50	50	-	-	-	-	-	-	no effect

**Table S7.** Results for sensitivity to shock for peroctanoic acid; (+) positive effect of experiment, (-) negative effect of experiment.

Weight / kg	Height / cm	Energy / J	No. of experiment						Observed effect
			1	2	3	4	5	6	
1	50	5	-						no effect
5	60	30	-						no effect
10	50	50	-	-	-	-	-	-	no effect

**Table S8.** Results for sensitivity to shock for perdecanoic acid; (+) positive effect of experiment, (-) negative effect of experiment.

Weight / kg	Height / cm	Energy / J	No. of experiment						Observed effect
			1	2	3	4	5	6	
1	50	5	-						no effect
5	60	30	-						no effect
10	50	50	-	-	-	-	-	-	no effect

**Table S9.** Results for sensitivity to shock for perdoecanoic acid; (+) positive effect of experiment, (-) negative effect of experiment.

Weight / kg	Height / cm	Energy / J	No. of experiment						Observed effect
			1	2	3	4	5	6	
1	50	5	-						no effect
5	60	30	-						no effect
10	50	50	-	-	-	-	-	-	no effect

## 5. Sensitivity of peracids to electric spark.

**Table S10.** Results for sensitivity to the electric spark for peroctanoic acid; (+) positive effect of experiment, (-) negative effect of experiment.

Energy / J	No. of experiment						Observed effect
	1	2	3	4	5	6	
13.50	-	+					smoke
11.76	+						smoke
10.14	+						smoke
6.00	+						smoke
4.50	+						smoke
4.21	-	-	+				smoke
3.92	+						smoke
3.65	+						smoke
3.38	+						smoke
2.88	+						smoke
2.00	+						smoke
1.96	+						smoke
1.00	+						smoke
0.54	-	+					smoke
0.62	+						smoke
0.56	-	-	-	-	-	-	no effect
0.52	-	-					no effect
0.49	-						no effect
0.42	-						no effect



**Table S11.** Results for sensitivity to the electric spark for perdecanoic acid; (+) positive effect of experiment, (-) negative effect of experiment.

Energy /J	No. of experiment						Observed effect
	1	2	3	4	5	6	
13.50	-	-	-	-	-	-	no effect in 6 experiments; in experiment no. 7 smoke was observed
12.615	-	-	-	-	-	-	no effect

**Table S12.** Results for sensitivity to the electric spark for perdocanoic acid; (+) positive effect of experiment, (-) negative effect of experiment.

Energy /J	No. of experiment						Observed effect
	1	2	3	4	5	6	
13.50	-	-	-	-	-	+	smoke
12.615	-	+					smoke
11.76	-	-	-	-	-	-	no effect

## 6. Thermal sensitivity of peracid.

**Table S13.** Results for thermal stability.

Peracid	Sample / mg	Rate of heating / °C/min	Melting				Decomposition			
			Temperature / °C			Heat / J/g	Temperature / °C			Heat / J/g
			Initial	Max.	End		Initial	Max.	End	
C <sub>8</sub>	3.0000	2	26.06	32.82	36.71	135.1	51.37	70.95	77.51	307.8
	2.7000	5	22.39	33.38	40.88	205.6	69.69	92.16	100.00	313.6
	2.0000	10	21.56	34.12	45.04	225.4	65.36	92.18	102.66	709.5
C <sub>10</sub>	2.9000	2	36.55	44.09	53.20	256.6	71.19	87.16	116.65	770.6
	3.4000	5	29.05	44.90	52.53	240.5	64.19	96.19	114.48	1036.0
	3.8000	10	29.55	45.57	58.36	255.3	77.51	104.12	130.64	1077.0
C <sub>12</sub>	3.0500	2	39.47	51.29	56.98	219.5	71.19	94.12	127.47	616.6
	3.0500	5	39.88	51.75	58.53	239.6	68.69	108.99	147.96	734.1
	3.2000	10	41.04	54.11	64.86	242.0	73.85	116.25	160.00	828.1