TABLE 1: Zero-point vibrational energies within the harmonic approximation of the most stable structures of the alkyl peroxyl radicals in electron volt.[a]

compd	method	Neutral	Anion
CH_3OO	B3LYP	1.165	1.112
	BLYP	1.120	1.067
	BHLYP	1.217	1.164
	B3PW91	1.171	1.117
	BPW91	1.130	1.075
	B3P86	1.173	1.119
	BP86	1.124	1.070
	MP2	1.198	1.149
C_2H_5OO	B3LYP	1.938	1.881
	BLYP	1.871	1.814
	BHLYP	2.018	1.960
	B3PW91	1.947	1.889
	BPW91	1.886	1.827
	B3P86	1.950	1.891
	BP86	1.876	1.817
	MP2	1.988	1.934
n-C_3H_7OO	B3LYP	2.714	2.654
	BLYP	2.625	2.564
	BHLYP	2.821	2.761
	B3PW91	2.726	2.665
	BPW91	2.645	2.582
	B3P86	2.729	2.668
	BP86	2.631	2.569
n-C_4H_9OO	B3LYP	3.487	3.425
	BLYP	3.374	3.314
	BHLYP	3.622	3.559
	B3PW91	3.501	3.437
	BPW91	3.399	3.335
	B3P86	3.504	3.441
	BP86	3.381	3.316
n-$C_5H_{11}OO$	B3LYP	3.443	3.375
	BLYP	3.331	3.265
	BHLYP	3.576	3.507
	B3PW91	3.456	3.385
	BPW91	3.354	3.283
	B3P86	3.459	3.388
	BP86	3.337	3.265
i-C_3H_7OO	B3LYP	4.258	4.195
	BLYP	4.123	4.063
	BHLYP	4.420	4.357

	B3PW91	4.275	4.210
	BPW91	4.152	4.087
	B3P86	4.278	4.214
	BP86	4.130	4.063
t-C_4H_9OO	B3LYP	2.698	2.635
	BLYP	2.608	2.546
	BHLYP	2.804	2.740
	B3PW91	2.709	2.644
	BPW91	2.628	2.562
	B3P86	2.712	2.647
	BP86	2.614	2.548

[a] Values are obtained with the DZP++ basis set.

TABLE 2: Total energies and ZPVE corrected total energies of the most stable structures of the alkyl peroxyl radicals in electron volt.[b]

compd	method	Total energy of neutral	Corrected Total energy of neutral	Total energy of anion	Corrected Total energy of anion
CH_3OO	B3LYP	-5177.556	-5176.392	-5178.603	-5177.491
	BLYP	-5176.584	-5175.465	-5177.599	-5176.532
	BHLYP	-5174.654	-5173.437	-5175.395	-5174.231
	B3PW91	-5175.512	-5174.341	-5176.418	-5175.301
	BPW91	-5177.176	-5176.046	-5178.114	-5177.039
	B3P86	-5189.527	-5188.354	-5191.016	-5189.897
	BP86	-5177.728	-5176.603	-5178.824	-5177.754
	MP2	-5162.754	-5161.556	-5163.858	-5162.710
C_2H_5OO	B3LYP	-6247.676	-6245.737	-6248.703	-6246.821
	BLYP	-6245.939	-6244.068	-6246.920	-6245.106
	BHLYP	-6244.075	-6242.057	-6244.807	-6242.847
	B3PW91	-6245.267	-6243.319	-6246.152	-6244.264
	BPW91	-6247.066	-6245.180	-6247.970	-6246.143
	B3P86	-6263.646	-6261.696	-6265.118	-6263.226
	BP86	-6247.771	-6245.895	-6248.836	-6247.019
	MP2	-6229.214	-6227.226	-6230.324	-6228.390
n-C_3H_7OO	B3LYP	-7317.625	-7314.910	-7318.668	-7316.013
	BLYP	-7315.119	-7312.494	-7316.113	-7313.548
	BHLYP	-7313.330	-7310.509	-7314.082	-7311.321
	B3PW91	-7314.851	-7312.125	-7315.754	-7313.089
	BPW91	-7316.781	-7314.136	-7317.698	-7315.116
	B3P86	-7337.595	-7334.867	-7339.088	-7336.420
	BP86	-7317.640	-7315.009	-7318.724	-7316.155
n-C_4H_9OO	B3LYP	-8387.584	-8384.097	-8388.645	-8385.220
	BLYP	-8384.313	-8380.938	-8385.338	-8382.024
	BHLYP	-8382.591	-8378.970	-8383.359	-8379.800

	B3PW91	-8384.444	-8380.943	-8385.365	-8381.928
	BPW91	-8386.505	-8383.106	-8387.451	-8384.116
	B3P86	-8411.556	-8408.052	-8413.067	-8409.626
	BP86	-8387.523	-8384.143	-8388.632	-8385.316
n-$C_5H_{11}OO$	B3LYP	-8387.844	-8384.401	-8388.842	-8385.467
	BLYP	-8384.574	-8381.243	-8385.505	-8382.240
	BHLYP	-8382.851	-8379.275	-8383.573	-8380.066
	B3PW91	-8384.698	-8381.242	-8385.568	-8382.183
	BPW91	-8386.759	-8383.404	-8387.632	-8384.349
	B3P86	-8411.837	-8408.378	-8413.303	-8409.915
	BP86	-8387.806	-8384.469	-8388.848	-8385.583
i-C_3H_7OO	B3LYP	-9457.543	-9453.285	-9458.610	-9454.414
	BLYP	-9453.505	-9449.382	-9454.544	-9450.481
	BHLYP	-9451.853	-9447.433	-9452.627	-9448.270
	B3PW91	-9454.037	-9449.762	-9454.965	-9450.755
	BPW91	-9456.230	-9452.078	-9457.185	-9453.098
	B3P86	-9485.516	-9481.237	-9487.033	-9482.819
	BP86	-9457.405	-9453.275	-9458.522	-9454.459
t-C_4H_9OO	B3LYP	-7317.788	-7315.090	-7318.820	-7316.185
	BLYP	-7315.285	-7312.677	-7316.269	-7313.723
	BHLYP	-7313.490	-7310.686	-7314.232	-7311.491
	B3PW91	-7315.010	-7312.301	-7315.905	-7313.261
	BPW91	-7316.941	-7314.313	-7317.853	-7315.291
	B3P86	-7337.765	-7335.053	-7339.252	-7336.605
	BP86	-7317.813	-7315.199	-7318.892	-7316.343

[b] Values are obtained with the DZP++ basis set.