Supporting Information

Reactivity of Triarylphosphine Peroxyl Radical Cations Generated through the Reaction of Triarylphosphine Radical Cations with Oxygen

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Figure S1. Transient absorption spectra observed at 50 ns, 500 ns, 1 μs , and 5 μs after an electron pulse during the pulse radiolysis of **1** (10 mM) in Ar-saturated PhCN. (A) **1a**, (B) **1b**, (C) **1c**, (D) **1d**, (E) **1e**, (F) **1g**, (G) **1h**, (H) **1i**, (J) **1k**, and (K) **1l**.

Figure S2. Transient absorption spectra observed at 50 ns, 500 ns, 1 μs, and 5 μs after an electron pulse during the pulse radiolysis of **1** (10 mM) in O₂-saturated PhCN. (A) **1d**, (B) **1h**.

Table S1. Cartesian Coordinates of **1f⁺**. (Total energy: -1153.637550 Hartree).^a

	Coordinates (Angstroms)		
	X	Y	Z
P	0.00071	-0.00045	-0.79163
C	-0.44245	1.67126	-0.33592
C	-1.22648	-1.21973	-0.33823
C	1.6693	-0.45334	-0.33461
C	-2.53122	-1.09675	-0.86605
C	-3.49693	-2.04524	-0.56029
C	-3.19953	-3.15005	0.25745
C	-1.8925	-3.27345	0.76005
C	-0.91281	-2.33335	0.46836
C	2.47275	0.37215	0.47941
C	3.77373	-0.00955	0.77996
C	4.32322	-1.20094	0.275
C	3.51737	-2.01079	-0.54498
C	2.21612	-1.64536	-0.85974
C	-1.55862	1.95504	0.4783
C	-1.87758	3.27289	0.77884
C	-1.12013	4.34389	0.27336
C	-0.01624	4.05011	-0.54677
C	0.31712	2.74022	-0.86118
C	-1.49785	5.76897	0.5778
C	-4.25854	-4.16293	0.6017
C	5.74621	-1.58556	0.58028
H	-2.78326	-0.26515	-1.51834
H	-4.49684	-1.93862	-0.97172
H	-1.64315	-4.11928	1.39504
H	0.08527	-2.45024	0.87739
H	2.07176	1.29142	0.8933
H	4.37565	0.62309	1.42669
H	3.9233	-2.93428	-0.94846
H	1.62293	-2.28072	-1.51168
H	-2.15453	1.14847	0.89234
H	-2.7261	3.47855	1.42575
H	0.581	4.86298	-0.95052
H	1.16416	2.54353	-1.51265
H	-2.19578	6.15016	-0.17965
H	-0.62347	6.42654	0.57382
H	-1.99348	5.85494	1.54933
H	-4.78906	-3.86679	1.51664
H	-3.82604	-5.15145	0.78229
H	-5.00511	-4.24987	-0.19326
H	6.06638	-1.20254	1.5538
H	6.42579	-1.16754	-0.17443
H	5.88032	-2.67129	0.57233

^a Calculated at UB3LYP/6-31Gd level.