Supporting Information for:

Trends in Ground-State Entropies for Transition Metal Based Hydrogen Atom Transfer Reactions

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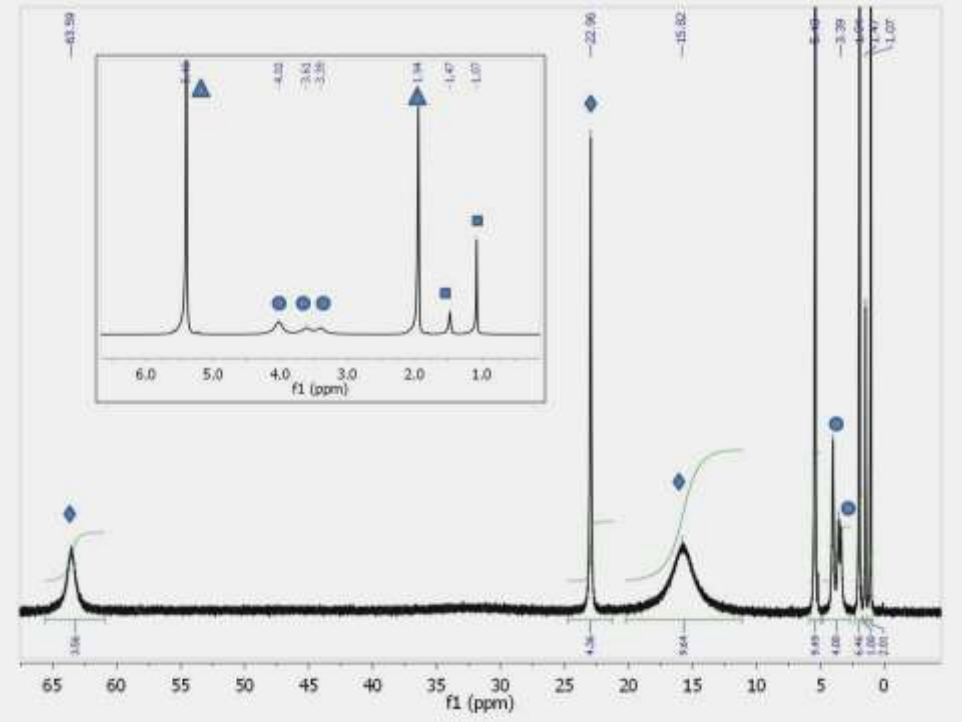

Figure S1. ^{1}H NMR spectrum of an equilibrium mixture of **$Co^{II}(H_2bim)$ (♦)** + TEMPO ⇄ **$Co^{III}(Hbim)$** (●) + TEMPOH **(■)** starting from 10.8 mM **$Co^{II}(H_2bim)$** and 0.12 M TEMPO in CD_3CN at 280K. The remaining peaks (▲) are residual solvent and CH_2Cl_2 (integration standard). Inset: Upfield region of spectrum.

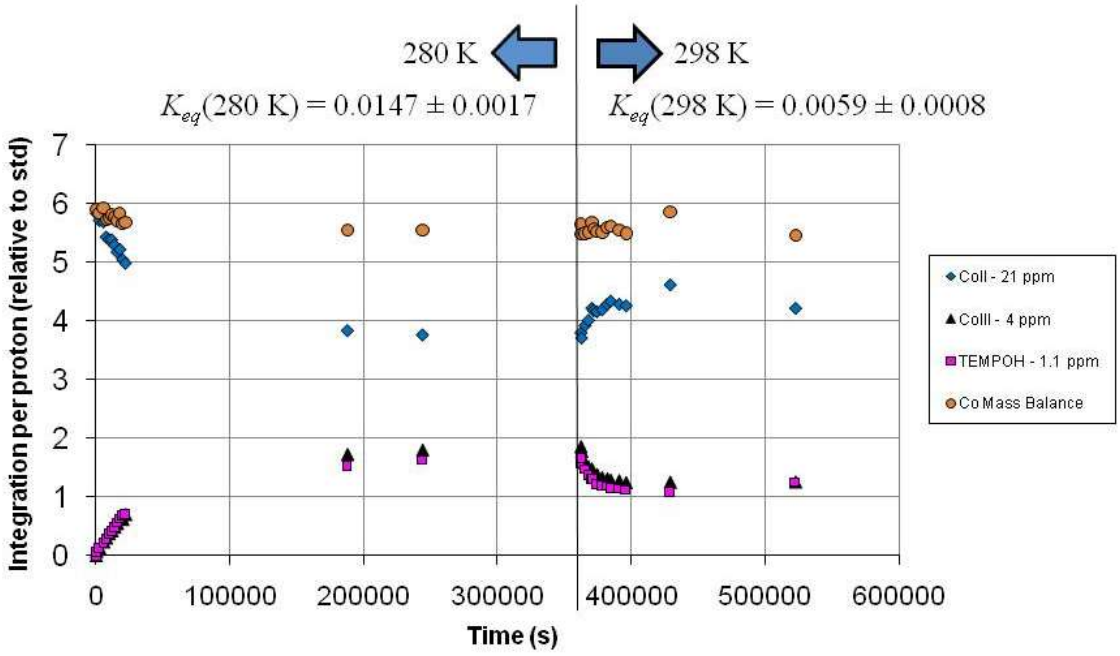

Figure S2. Equilibration study for **$Co^{II}(H_2bim)$** + TEMPO ⇄ **$Co^{III}(Hbim)$** + TEMPOH. Mixed 10.8 mM **$Co^{II}(H_2bim)$** and 0.12 M TEMPO in CD_3CN and plotted change in integration of ^1H NMR signal versus time. For the first 36000 seconds the reaction was equilibrated at 280 K, then the NMR tube was removed from the cold bath and re-equilibrated at 298 K (36000 to 52000 seconds). The appearance of TEMPOH (■) and **$Co^{III}(Hbim)$** (▲)are plotted along with the dissappearance of **$Co^{II}(H_2bim)$** (♦) and total amount of cobalt (●).

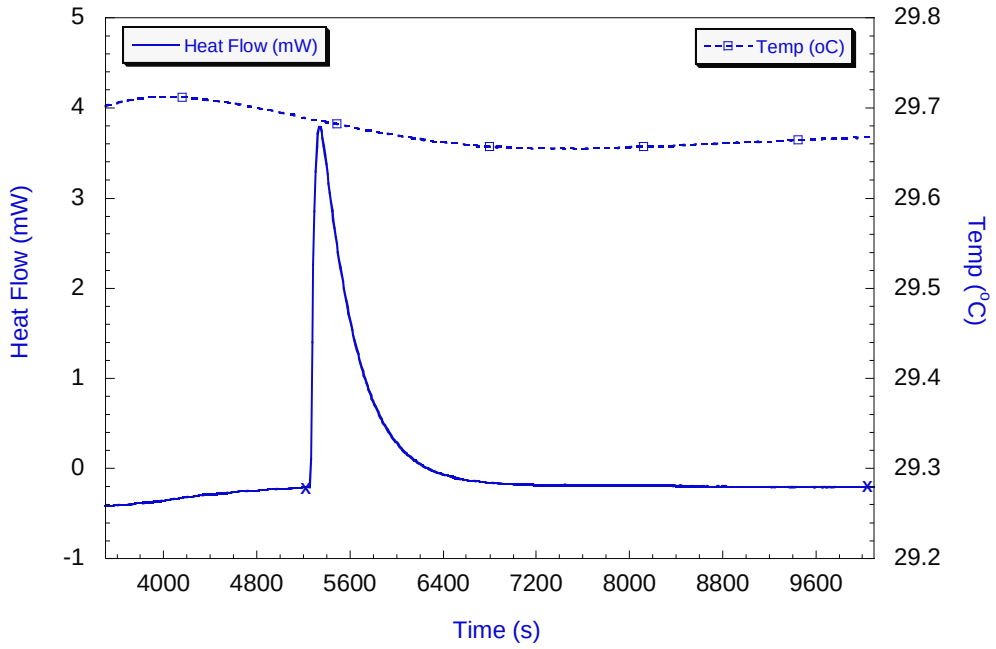

Figure S3. Heat flow curve (**—**) and sample temperature (-□-) for the reaction between 11.0 mM TEMPOH + 14.7 mM $^{t}Bu_3PhO^{\bullet}$ in MeCN. The "x" mark the integration points used to extract the enthalpy of reaction.

BDFE[TEMPOH]$_{MeCN}$ determination from pK_a and E° values.

Figure S4 shows the relevant values required to determine the BDFE of TEMPOH in MeCN using a pK_a and E° thermochemical cycle. Equation 21 from the text is reproduced here for clarity as eq S1. E°[TEMPOH] is a reversible wave at 0.71 V vs $FeCp_2^{+/0}$.[1] E°[TEMPOH$^{+\bullet}$] is an irreversible wave at -1.9 V vs $FeCp_2^{+/0}$.[2] The pK_a for TEMPOH was measured in DMSO by Bordwell and co-workers[3] and can be converted to a value in MeCN using the linear relation discovered for phenols by Chantooni[4] and generalized to other substrates by Kutt.[5] The pK_a[TEMPOH$^{+\bullet}$] is determined from eq S2 (all potentials in V vs. $Fc^{+/0}$) to be -3. This very low pK_a is consistent with the literature indicating that TEMPO$^{+\bullet}$ should be a very acidic species.[6]

$$\mathrm{BDFE_{MeCN}\ (kcal\ mol^{-1})} = nFE^\circ(\mathrm{vs.\ Fc^{+/0}}) + 2.303RT\mathrm{p}K_a + 54.9 \qquad \text{(S1)}$$

$$23.1\{E^\circ[\mathrm{TEMPOH}] - E^\circ[\mathrm{TEMPO^-}]\} = 1.37\{\mathrm{p}K_a[\mathrm{TEMPOH}] - \mathrm{p}K_a[\mathrm{TEMPO^{+\bullet}}]\} \qquad \text{(S2)}$$

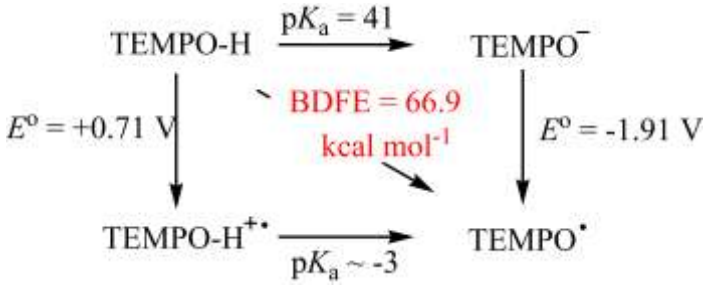

Figure S4. Thermochemical data for TEMPOH in MeCN.

Calculations

Unless stated otherwise all data was generated using the (RO)B3LYP/6-31+G(,p) method, following Bakalbassis.[7] Bakalbassis found this method to give comparable results to his preferred method, (U)B3LYP/6-31+(,3pd), which was too computationally costly for the ^{t}Bu$_3$PhO$^\bullet$/H system. For PCM calculations on hydrogen atom, the atomic radius reported by Bondi[8] was used in the creation of the cavity. However, $\Delta H_{solv}[H^\bullet]_{MeCN}$ was computed to be very small, < 0.1 kcal mol^{-1}, therefore the experimental estimate, $\Delta H_{solv}[H^\bullet]_{MeCN} \approx \Delta H_{solv}[H_2]_{MeCN}$ = 1.56 kcal mol^{-1}, was used in conjunction with the computational value of ΔH_{solv} [^{t}Bu$_3$PhO$^\bullet$ – ^{t}Bu$_3$PhOH] in Eq. 19 for the computation of BDE[^{t}Bu$_3$PhOH]$_{MeCN}$.

Preliminary geometry optimizations were performed at (U)/B3LYP/6-31G(d) and (U)B3LYP/6-31+G(,p) levels of theory. Computed values of BDE, ΔH°_{solv} [^{t}Bu$_3$PhO$^\bullet$ – ^{t}Bu$_3$PhOH], and ΔG°_{solv} are given in Table S6. The effect of the solvent model on the optimized geometries was chemically negligible. Selected bond lengths are given in Table S7. Relevant computed electronic and thermochemical data are given in Table S8.

Cartesian coordinates for (RO)B3 LYP/6-31+G(,p) optimized structures are given in Tables S9-S12.

Table S6. Computed BDE's, $\Delta H°_{solv}$ [$^{t}Bu_3PhO^{\cdot}$ – $^{t}Bu_3PhOH$], and $\Delta G°_{solv}$.[a]

	(RO)B3LYP/6-31+G(,p)
$BDE_{(g)}$[b,c]	79.3
$BDE_{(MeCN)}$[c]	78.9
$\Delta H°_{solv}$ [$^{t}Bu_3PhO^{\cdot}$ – $^{t}Bu_3PhOH$][d]	-0.4
$\Delta G°_{solv,MeCN}$ [$^{t}Bu_3PhO^{\bullet}_{(g)}$ – $^{t}Bu_3PhOH_{(g)}$][e]	-0.4
$\Delta G°_{solv,C6H6}$ [$^{t}Bu_3PhO^{\bullet}_{(g)}$ – $^{t}Bu_3PhOH_{(g)}$][e]	+.04

[a] All energies are in kcal mol^{-1}. [b] The experimental value is BDE[$^{t}Bu_3PhOH_{(g)}$] = 79.9 kcal mol^{-1}, see manuscript. [c] Here BDE is calculated from absolute enthalpies, BDE = H_{DFT}[$^{t}Bu_3PhO^{\bullet}_{(g)}$] + H_{DFT}[$H^{\bullet}_{(g)}$] – H_{DFT}[$^{t}Bu_3PhOH_{(g)}$]. [d] $\Delta H°_{solv}$[$^{t}Bu_3PhO^{\bullet}$ – $^{t}Bu_3PhOH$] = H_{DFT}[$^{t}Bu_3PhOH_{(sln)}$] + H_{DFT}[$^{t}Bu_3PhO^{\bullet}_{(g)}$] – H_{DFT}[$^{t}Bu_3PhOH_{(g)}$] – H_{DFT}[$^{t}Bu_3PhO^{\bullet}_{(sln)}$]. [e] $\Delta G°_{solv}$ values for $^{t}Bu_3PhOH$ and $^{t}Bu_3PhO^{\bullet}$ were obtained from PCM single point calculations, see above.

Table S7. Selected bond lengths (Å) optimized at (RO)B3LYP/6-31+G(,p) with and without acetonitrile solvent model.

	ArOH		ArO$^{\bullet}$	
Distance	gas	MeCN	gas	MeCN
C1,O	1.412	1.411	1.293	1.295
C1, C2	1.414	1.415	1.465	1.468
C2,C3	1.410	1.411	1.392	1.391
C3,C4	1.400	1.400	1.412	1.413
C1,C2'	1.416	1.418	1.467	1.469
C2',C3'	1.402	1.403	1.386	1.385
C3',C4	1.406	1.406	1.419	1.420

Table S8. Computed electronic and thermochemical data.[a]

		(RO)B3LYP/6-31+G(,p)	
		Gas Phase	Solution[b]
^{t}Bu$_3$PhOH	$E_{el,DFT}$[c]	-779.12467	-779.12892
	$E_{el,DFT}$ + ZPE[d]	-778.68111	-778.68629
	H_{DFT}[e]	-778.65822	-778.66339
	G_{DFT}[f]	-778.72916	-778.73415
	Dipole[g]	2.055	2.4532
	$\Delta G_{solv(MeCN)}$[h]		8.2
	$\Delta G_{solv(C6H6)}$[h,i]		2.4
^{t}Bu$_3$PhO$^\bullet$	$E_{el,DFT}$	-778.48708	-778.49501
	$E_{el,DFT}$ + ZPE	-778.05655	-778.06234
	H_{DFT}	-778.03399	-778.03975
	G_{DFT}	-778.10546	-778.11114
	Dipole	3.939	5.413
	$\langle S^2 \rangle$	NA	NA
	$\Delta G_{solv(MeCN)}$[h]		7.8
	$\Delta G_{solv(C6H6)}$[h,i]		2.4
H$^\bullet$	$E_{el,DFT}$	-0.50027	-0.50049
	$E_{el,DFT}$ + ZPE	-0.50027	-0.50049
	H_{DFT}	-0.49791	-0.49813
	G_{DFT}	-0.51093	-0.51114

[a] Energies are in hartrees, unless otherwise noted. [b] Computed with PCM model, see Experimental Section. Unless stated otherwise, the solvent is acetonitrile. [c] Electronic energy. [d] Sum of electronic and zero-point vibrational energies. [e] Sum of electronic and thermal enthalpies. [f] Sum of electronic and thermal free energies. [g] Total dipole in Debye. [h] Free energy of solution (kcal mol^{-1}) is computed on the gas-phase optimized geometry, using the SCFVAC keyword in Gaussian 03, see Experimental Section. [i] Solvent = benzene.

Table S9. Cartesian coordinates for $^{t}Bu_3PhOH$ optimized at B3LYP/6-31+G(,p), gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Å) X	Y	Z
1	8	0	2.596043	0.565818	0.000260
2	6	0	1.225845	0.226711	0.000115
3	6	0	0.792415	-1.118866	0.000042
4	6	0	0.324101	1.319096	-0.000011
5	6	0	-0.599025	-1.344905	0.000015
6	6	0	-1.043916	1.011971	-0.000102
7	6	0	-1.535644	-0.305023	-0.000052
8	6	0	-3.060092	-0.551970	-0.000128
9	6	0	1.782249	-2.316466	0.000042
10	6	0	0.812936	2.789581	0.000012
11	6	0	1.043834	-3.681656	-0.000175
12	6	0	-0.370767	3.790812	-0.000331
13	6	0	2.667276	-2.306153	1.285791
14	6	0	1.658247	3.078532	1.275663
15	6	0	2.667580	-2.305858	-1.285490
16	6	0	1.658844	3.078372	-1.275280
17	6	0	-3.694019	0.090490	1.267397
18	6	0	-3.693838	0.090337	-1.267821
19	6	0	-3.414138	-2.058855	-0.000056
20	1	0	-1.753428	1.825640	-0.000183
21	1	0	-0.952591	-2.362095	0.000043
22	1	0	-4.777530	-0.072952	1.274797
23	1	0	-3.273920	-0.350869	2.176941
24	1	0	-3.516851	1.169011	1.304559
25	1	0	-4.502287	-2.178533	-0.000132
26	1	0	-4.777352	-0.073082	-1.275349
27	1	0	-3.025543	-2.567396	0.888245
28	1	0	-3.516630	1.168849	-1.305090
29	1	0	-3.025415	-2.567518	-0.888232
30	1	0	-3.273622	-0.351149	-2.177249
31	1	0	1.784901	-4.487074	0.000091
32	1	0	0.028499	4.809692	-0.000152
33	1	0	0.418006	-3.807441	0.888025
34	1	0	-1.000115	3.682805	0.888885
35	1	0	0.418619	-3.807473	-0.888797
36	1	0	-0.999524	3.682891	-0.889975
37	1	0	3.356272	-3.157351	1.271564
38	1	0	1.986000	4.124466	1.272288
39	1	0	2.035356	-2.392416	2.174804
40	1	0	1.058081	2.915285	2.177578
41	1	0	3.266751	-1.400252	1.412638
42	1	0	2.538743	2.438698	1.321658
43	1	0	3.356858	-3.156826	-1.271103
44	1	0	1.986627	4.124296	-1.271862
45	1	0	2.035885	-2.392370	-2.174640
46	1	0	1.059086	2.915051	-2.177452
47	1	0	3.266673	-1.399697	-1.412147
48	1	0	2.539341	2.438506	-1.320818
49	1	0	3.159440	-0.214154	0.001189

Table S10. Cartesian coordinates for $^{t}Bu_3PhOH$ optimized at B3LYP/6-31+G(,p), MeCN solution..

Center Number	Atomic Number	Atomic Type	Coordinates (Å) X	Y	Z
1	8	0	-2.591983	0.606022	-0.001209
2	6	0	-1.229024	0.242399	-0.000367
3	6	0	-0.811501	-1.109403	0.000194
4	6	0	-0.310332	1.323185	-0.000388
5	6	0	0.578355	-1.350865	0.000278
6	6	0	1.054530	0.999666	-0.000502
7	6	0	1.529597	-0.323690	-0.000259
8	6	0	3.050931	-0.590484	-0.000209
9	6	0	-1.810321	-2.299891	0.000547
10	6	0	-0.775141	2.802192	-0.000116
11	6	0	-1.081532	-3.670690	0.001954
12	6	0	0.423624	3.785823	0.000934
13	6	0	-2.694859	-2.282947	-1.284557
14	6	0	-1.614491	3.106302	-1.276091
15	6	0	-2.696251	-2.281151	1.284674
16	6	0	-1.615847	3.105373	1.275223
17	6	0	3.693911	0.045977	-1.266447
18	6	0	3.693140	0.043205	1.267825
19	6	0	3.385633	-2.101849	-0.001846
20	1	0	1.774480	1.804171	-0.000643
21	1	0	0.918905	-2.372437	0.000650
22	1	0	4.775380	-0.130576	-1.270740
23	1	0	3.271630	-0.391926	-2.177136
24	1	0	3.529455	1.126825	-1.302955
25	1	0	4.472445	-2.233784	-0.002263
26	1	0	4.774655	-0.133065	1.272345
27	1	0	2.990350	-2.604761	-0.890588
28	1	0	3.528350	1.123902	1.306614
29	1	0	2.990838	-2.606671	0.886024
30	1	0	3.270405	-0.396767	2.177296
31	1	0	-1.830820	-4.468373	0.002442
32	1	0	0.038701	4.810445	0.001224
33	1	0	-0.457479	-3.803332	-0.886856
34	1	0	1.051873	3.668346	-0.887860
35	1	0	-0.457970	-3.801725	0.891348
36	1	0	1.050971	3.667458	0.890248
37	1	0	-3.381200	-3.136176	-1.272886
38	1	0	-1.932127	4.155461	-1.268094
39	1	0	-2.063956	-2.363797	-2.175299
40	1	0	-1.012558	2.942656	-2.177063
41	1	0	-3.300609	-1.379457	-1.400445
42	1	0	-2.499750	2.473211	-1.328001
43	1	0	-3.382516	-3.134444	1.273464
44	1	0	-1.933398	4.154560	1.267642
45	1	0	-2.066300	-2.360715	2.176206
46	1	0	-1.014851	2.941059	2.176701
47	1	0	-3.302189	-1.377555	1.398684
48	1	0	-2.501196	2.472315	1.325771
49	1	0	-3.188185	-0.151941	-0.001251

Table S11. Cartesian coordinates for $^{t}Bu_3PhO^{\bullet}$ optimized at ROB3LYP/6-31+G(,p), gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Å) X	Y	Z
1	8	0	-2.525670	0.611912	0.000352
2	6	0	-1.271019	0.299090	0.000159
3	6	0	-0.861947	-1.107954	0.000177
4	6	0	-0.248909	1.351990	-0.000046
5	6	0	0.499590	-1.397348	0.000004
6	6	0	1.082469	0.966694	-0.000201
7	6	0	1.493217	-0.392449	-0.000178
8	6	0	2.997266	-0.719354	-0.000349
9	6	0	-1.926594	-2.220744	0.000367
10	6	0	-0.667566	2.834534	-0.000073
11	6	0	-1.289768	-3.633272	0.000300
12	6	0	0.558671	3.781377	-0.000320
13	6	0	-2.818921	-2.105254	-1.273023
14	6	0	-1.509577	3.150319	-1.273532
15	6	0	-2.818535	-2.105196	1.274023
16	6	0	-1.509193	3.150473	1.273601
17	6	0	3.658361	-0.104987	-1.270301
18	6	0	3.658664	-0.104922	1.269415
19	6	0	3.278552	-2.241182	-0.000343
20	1	0	1.849001	1.727420	-0.000346
21	1	0	0.813454	-2.428280	0.000014
22	1	0	4.731176	-0.324935	-1.274619
23	1	0	3.218755	-0.525811	-2.180043
24	1	0	3.537846	0.980871	-1.307403
25	1	0	4.359705	-2.409886	-0.000455
26	1	0	4.731476	-0.324891	1.273502
27	1	0	2.868221	-2.731642	-0.888585
28	1	0	3.538179	0.980940	1.306477
29	1	0	2.868409	-2.731597	0.888011
30	1	0	3.219258	-0.525681	2.179283
31	1	0	-2.087990	-4.381543	0.000413
32	1	0	0.207154	4.817355	-0.000269
33	1	0	-0.675678	-3.807917	-0.889347
34	1	0	1.181991	3.645100	-0.890243
35	1	0	-0.675444	-3.807902	0.889788
36	1	0	1.182332	3.645130	0.889369
37	1	0	-3.555949	-2.915837	-1.275835
38	1	0	-1.783317	4.211242	-1.276573
39	1	0	-2.212221	-2.197275	-2.180674
40	1	0	-0.929566	2.948654	-2.180928
41	1	0	-3.345303	-1.151460	-1.294448
42	1	0	-2.420608	2.552829	-1.296369
43	1	0	-3.555570	-2.915772	1.277091
44	1	0	-1.782963	4.211387	1.276577
45	1	0	-2.211558	-2.197189	2.181492
46	1	0	-0.928895	2.948952	2.180845
47	1	0	-3.344899	-1.151395	1.295571
48	1	0	-2.420198	2.552957	1.296796

Table S12. Cartesian coordinates for $^{t}Bu_3PhO^{\bullet}$ optimized at ROB3LYP/6-31+G(,p) in MeCN solution.

Center Number	Atomic Number	Atomic Type	Coordinates (Å) X	Y	Z
1	8	0	-2.502060	0.739787	0.002355
2	6	0	-1.262228	0.365338	0.001070
3	6	0	-0.921337	-1.061735	0.000121
4	6	0	-0.187030	1.366776	0.000393
5	6	0	0.423699	-1.416455	0.000342
6	6	0	1.122736	0.915274	0.000459
7	6	0	1.467215	-0.462814	0.000729
8	6	0	2.950889	-0.867077	0.000549
9	6	0	-2.031426	-2.129972	-0.000727
10	6	0	-0.521718	2.871188	-0.000305
11	6	0	-1.453127	-3.568112	-0.001519
12	6	0	0.755260	3.749863	-0.003915
13	6	0	-2.915938	-1.982333	-1.275603
14	6	0	-1.343042	3.235098	-1.273632
15	6	0	-2.916572	-1.982407	1.274191
16	6	0	-1.338129	3.236655	1.276027
17	6	0	3.642882	-0.287344	-1.269886
18	6	0	3.643849	-0.287663	1.270513
19	6	0	3.150794	-2.401416	0.000190
20	1	0	1.926092	1.636097	0.000159
21	1	0	0.686672	-2.461150	0.000060
22	1	0	4.701169	-0.568875	-1.272793
23	1	0	3.180050	-0.683260	-2.179618
24	1	0	3.585257	0.803960	-1.304405
25	1	0	4.221960	-2.624904	0.000755
26	1	0	4.702110	-0.569344	1.272518
27	1	0	2.716343	-2.868600	-0.889416
28	1	0	3.586547	0.803634	1.305471
29	1	0	2.714989	-2.869166	0.888829
30	1	0	3.181691	-0.683730	2.180496
31	1	0	-2.282769	-4.281566	-0.002287
32	1	0	0.458923	4.803229	-0.004186
33	1	0	-0.846330	-3.766473	-0.891042
34	1	0	1.368742	3.579724	-0.894730
35	1	0	-0.846937	-3.767750	0.888128
36	1	0	1.372743	3.581331	0.884435
37	1	0	-3.686538	-2.761101	-1.276161
38	1	0	-1.557933	4.309450	-1.274691
39	1	0	-2.311154	-2.104464	-2.180985
40	1	0	-0.772467	3.003254	-2.179765
41	1	0	-3.400805	-1.006667	-1.304913
42	1	0	-2.284979	2.687485	-1.301134
43	1	0	-3.687441	-2.760911	1.274290
44	1	0	-1.553766	4.310857	1.276362
45	1	0	-2.312058	-2.105027	2.179700
46	1	0	-0.763562	3.006590	2.180111
47	1	0	-3.401132	-1.006583	1.303660
48	1	0	-2.279594	2.688481	1.308327

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