Electronic Supplementary Information (ESI)

Revisiting the Radical Trapping Activity of N-H and O-H in N-Phenylhydroxylamine: A DFT Study

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Table S1. Benchmark of the calculated BDE(N-H)s and BDE(O-H)s for substituted anilines and hydroxylamines using M062X/6-311++G(d,p) method in gas phase.

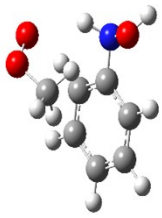
Compounds		BDE (calc.) kcal/mol	BDE (expt.) kcal/mol	ΔBDE
Phenol	O-H	87.8	88.0	-0.2
$(Et)_2NOH$	O-H	68.2	69.5	-1.3
$PhCH_2CH_2C(O)$ (tBu)NO–**H**	O-H	77.5	76.1	1.4
$CH_3(CH_2)_9C(O)$ (tBu)NO–**H**	O-H	75.0	75.8	-0.8
C(O)CHCHPh (tBu)NO–**H**	O-H	77.2	76.8	0.4
4-$NO_2C_6H_4$ (tBu)NO–**H**	O-H	78.8	80.2	-1.4
Aniline	N-H	89.5	89.7	-0.2
o-CF_3- Aniline	N-H	92.7	92.5	0.2
o-CH_3- Aniline	N-H	89.3	90.6	-1.3
o-CN- Aniline	N-H	93.1	95.1	-2.0
m-CF_3- Aniline	N-H	91.8	93.2	-1.4
m-Cl- Aniline	N-H	90.9	92.6	-1.7
p-CF_3- Aniline	N-H	91.9	92.0	-0.1
p-CH_3- Aniline	N-H	88.1	88.7	-0.6
p-CN- Aniline	N-H	92.4	91.8	0.6
p-F- Aniline	N-H	88.5	88.8	-0.3
$\Delta BDE = BDE_{calc.} - BDE_{expt.}$				

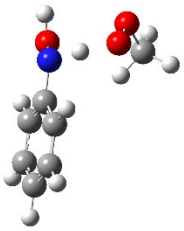
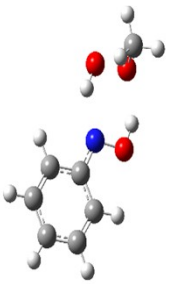
Table S2. Hammett plots for the BDEs of N-H and O-H

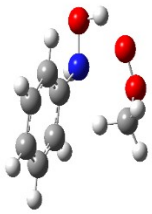
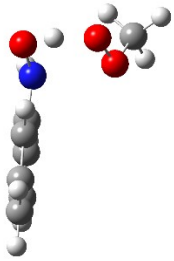
Substituent	Hammett value* σ^{+}_{p}	BDE(N-H), kcal/mol				BDE(O-H), kcal/mol			
		Gas phase	DMSO	water	ethanol	Gas phase	DMSO	water	ethanol
H	0	74.8	77.1	77.4	76.5	69.8	69.6	71.4	70.1
F	-0.07	74	76.6	77	75.9	69.8	69.6	71.4	70.0
Cl	0.11	74.5	77.3	77.6	76.6	70.1	70	71.9	70.6
CH_3	-0.31	74	76.1	75.9	75.5	69.3	69.1	70.2	69.4
OCH_3	-0.78	72.5	74.5	75.2	74.0	68.5	68.5	70.1	68.8
NH_2	-1.3	71.4	72.6	73.1	72.1	68.1	67.7	68.9	67.7
CF_3	0.61	76.1	79	79.3	78.2	71.1	71	72.5	71.7
CN	0.66	75.9	77.9	78.5	78.4	71.3	71.1	72.5	72.1
NO_2	0.79	76.6	80	80.5	79.4	71.8	71.9	73.4	73.0

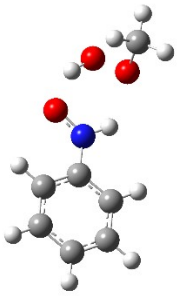
* Hansch, Corwin, A. Leo, and R. W. Taft. "A survey of Hammett substituent constants and resonance and field parameters." Chemical reviews 91.2 (1991): 165-195.

Table S3. Cartisian coordinates of RC, TS, PC in reaction of ArNHOH derivatives + $CH_3OO^{\bullet}$ in the gas phase and ethanol

S3A. ArNHOH + $CH_3COO^{\bullet}$ in the gas phase	
S3A1. Reaction at N-H bond	
RC at NH in gas phase 	C 0.56925600 0.67372200 -0.47622200 C 0.77024300 -0.51513400 -1.18584100 C 1.79551000 -1.37448900 -0.82049400 C 2.63247800 -1.06463400 0.25062900 C 2.43000600 0.12070500 0.94722200 C 1.40435300 0.99339800 0.59241000 H 0.11048900 -0.76336300 -2.01009900 H 1.93827100 -2.29599200 -1.37256600 H 3.07306800 0.37407100 1.78219600 H 1.23562800 1.90577200 1.14764600 N -0.47784800 1.52160300 -0.89692500 H -1.28265400 0.95936300 -1.16549400 O -0.92130800 2.36763200 0.14230100 H -0.83860300 3.25289800 -0.22319500 O -2.42170400 -0.87432000 -0.75800700 O -2.55627000 -1.37978200 0.42588500 C -1.70176800 -0.74122100 1.39622100 H -1.78395100 0.34086100 1.28910600 H -2.06777400 -1.07733500 2.36389600 H -0.67584800 -1.07058300 1.22661300 H 3.43009900 -1.73923700 0.53539100
TS at NH in gas phase 1 imaginary frequencies ignored. (-1900.92) Distance (D): D(HO**N**....**H**)= 1.14690 Å D(**H**...**O**OCH_3)= 1.31840 Å Angle (∠) ∠(HO)**N-H-O**(OCH_3) = 160.72369 °	C 0.68824600 0.16638200 -0.54051100 C 1.28007400 -1.10108600 -0.62746400 C 2.51394300 -1.32520300 -0.04161600 C 3.17321600 -0.29563300 0.63000900 C 2.58181900 0.96056200 0.71152100 C 1.33998500 1.20159200 0.13565300 H 0.75793500 -1.89465400 -1.15024000 H 2.96599600 -2.30748200 -0.10760200 H 4.14008500 -0.47362700 1.08413300 H 3.09107900 1.76512200 1.22877600 H 0.87781500 2.17721900 0.19265800 N -0.53723300 0.33652100 -1.19474700 H -1.26683400 -0.51298500 -0.94693600 O -1.14883700 1.50941100 -0.78920200 H -1.86784000 1.63663500 -1.41746600

	O -2.18591500 -1.22115700 -0.32087500 O -3.01422600 -0.29005800 0.20949500 C -2.64917200 -0.06270100 1.56644500 H -3.34973900 0.68328800 1.93946700 H -2.73869200 -0.99365800 2.12864200 H -1.62601200 0.31544800 1.61222700
PC at NH in gas phase 	C -0.94345800 -0.05602800 -0.08572200 C -1.49273000 1.23792700 0.01148100 C -2.85817300 1.40171800 0.15301600 C -3.69667200 0.28671400 0.20066500 C -3.15599400 -0.99617600 0.10506600 C -1.79133900 -1.18075000 -0.03754000 H -0.82381000 2.08967700 -0.02710100 H -1.36415000 -2.17095600 -0.11404500 N 0.41862200 -0.12073300 -0.22405000 H 1.95245800 0.96927600 -0.69851600 O 0.84868600 -1.39623500 -0.30486800 H 1.81689000 -1.29842300 -0.36974200 O 2.92227100 1.01114400 -0.82361100 O 3.31515900 -0.21266500 -0.21806100 C 3.76969300 0.08417400 1.09098000 H 4.11721700 -0.86535100 1.49993500 H 4.59268600 0.79857700 1.04362400 H 2.95367600 0.48303100 1.69961100 H -4.76621900 0.41698100 0.31113100 H -3.27612400 2.39830900 0.22683100 H -3.80987200 -1.85941500 0.14126700
S3A2. Reaction at O-H bond	
RC at OH in gas phase	C -0.35312700 0.91491300 -0.25756900 C -0.57745500 0.57728600 1.07691900 C -2.61912600 -0.56583000 0.44933700 C -1.26696000 0.51004500 -1.23822200 H 0.13231500 0.89026400 1.82952500 H -1.07760300 0.75762200 -2.27750500 N 0.82098500 1.56589000 -0.68163200 H 0.63788000 2.33264300 -1.31838300 O 1.59868600 2.07689200 0.36404600

	H 2.31075600 1.42738300 0.44319600 O 2.25175700 -0.70245600 0.62023000 O 1.93022000 -1.26433200 -0.50085800 C 0.95912100 -2.30977100 -0.31097100 H 1.33964900 -3.00746800 0.43397000 H 0.02062400 -1.85868200 0.01365400 H 0.85197800 -2.78351700 -1.28409900 C -2.39102800 -0.22007800 -0.88253600 C -1.70878200 -0.15985700 1.41837800 H -1.87591200 -0.41588400 2.45834000 H -3.49612100 -1.13841600 0.72412200 H -3.09161600 -0.52624600 -1.65076200
TS at OH in gas phase OK **1 imaginary frequencies ignored.** (**-1259.51cm^{-1}**) **Distance (D):** D(HN**O....H**)= **1.07097** Å D(**H...O**OCH_3)= **1.35171** Å **Angle** (∠) ∠(HN)**O-H-O**(OCH_3) = **162.78818** ° 	C -0.69442100 0.12634500 0.55744700 C -1.53501100 1.24119000 0.47315500 C -2.76640100 1.12568800 -0.15257600 C -3.16780400 -0.09060100 -0.70080500 C -2.32197100 -1.19228800 -0.61476900 C -1.08454600 -1.09568200 0.00774400 H -1.22066700 2.18851200 0.89892600 H -3.41718500 1.98991200 -0.21130100 H -4.13022200 -0.17721500 -1.18913100 H -2.62609500 -2.14144100 -1.03968000 H -0.42131100 -1.94728400 0.07590600 N 0.56009900 0.27370200 1.14255600 H 0.72287300 1.07663400 1.73702900 O 1.25100400 -0.80800700 1.51862000 H 1.86069300 -1.06676000 0.67701900 O 2.49504700 -1.03526200 -0.51618500 O 2.07138600 0.14707200 -0.98872700 C 3.05560600 1.14536800 -0.73815500 H 3.96356500 0.90310100 -1.29250600 H 2.62522000 2.08258800 -1.08772200 H 3.27023600 1.18549000 0.33165000

PC at OH in gas phase 	C 1.00130000 -0.07029500 -0.05509400 C 1.83551400 -1.15781000 0.20919900 C 3.20535600 -0.94975700 0.27518700 C 3.74292000 0.32117200 0.08102700 C 2.89874800 1.39751100 -0.18331300 C 1.52673700 1.20930800 -0.25296800 H 1.39456800 -2.13471700 0.35583500 H 0.86220800 2.04102300 -0.46158300 N -0.38153100 -0.24444600 -0.12817500 H -1.00151100 0.55415900 -0.29231300 O -0.94658300 -1.36855100 0.03989200 H -2.68019400 -1.09131000 -0.67112200 O -3.39696300 -0.48089200 -0.93130000 O -3.03110800 0.68660000 -0.21022500 C -3.73898800 0.66995200 1.01517600 H -4.81289500 0.62424500 0.82655700 H -3.42508200 -0.17913800 1.62908200 H -3.48419600 1.60739900 1.51152300 H 3.31092900 2.38728600 -0.33707600 H 4.81384800 0.47217000 0.13422500 H 3.86075800 -1.78772500 0.47988200
S3B. ArNHOH + $CH_3COO^{\bullet}$: in ethanol	
S3D1. ArNHOH + $CH_3COO^{\bullet}$ at the N-H bond in ethanol	
RC at NH in ethanol	0 2 C 0.60355300 0.67246200 -0.46135200 C 0.79781700 -0.50218100 -1.19820000 C 1.80275900 -1.38834400 -0.83700500 C 2.62613100 -1.11956700 0.25735300 C 2.43141100 0.05249500 0.98021100 C 1.42682700 0.95261600 0.62857300 H 0.15299600 -0.71488300 -2.04497500 H 1.94091000 -2.29807600 -1.41088100 H 3.06433300 0.27551500 1.83232000 H 1.27659800 1.85891600 1.20063000 N -0.40932700 1.55667400 -0.88982800 H -1.22419400 1.03102300 -1.20122500 O -0.85478800 2.40771800 0.14144000 H -0.66344500 3.30026600 -0.17138500 O -2.45462700 -0.85723500 -0.78499700 O -2.66531600 -1.32338200 0.40342900 C -1.77826600 -0.74679000 1.38815700 H -1.81572800 0.33883000 1.29924300

	H -2.16380100 -1.08162300 2.34892700 H -0.77347700 -1.13231500 1.21139600 H 3.40754400 -1.81531700 0.53933600
TS at NH in ethanol 1 imaginary frequencies ignored. (-2545.8155cm^{-1}) Distance (D): D(HO**N**....**H**)= <u>1.12380</u> Å D(**H**...**O**OCH_3)= <u>1.37198</u> Å Angle (∠) ∠(HO)**N-H-O**(OCH_3) = <u>159.08325</u> °	0 2 C 0.66133100 0.26535200 -0.52921600 C 1.22264700 -0.99234300 -0.79442400 C 2.44622700 -1.32869800 -0.23856100 C 3.12259000 -0.42176500 0.57917900 C 2.56056700 0.82591800 0.83612100 C 1.33033600 1.17846900 0.29177400 H 0.68910100 -1.69018100 -1.43149500 H 2.87605800 -2.30257200 -0.44302100 H 4.08051900 -0.68743400 1.01057400 H 3.08305600 1.53568300 1.46749700 H 0.89714700 2.14976200 0.48997900 N -0.55253500 0.55855200 -1.16231100 H -1.27925800 -0.29444500 -1.07745300 O -1.15715400 1.66676600 -0.61113600 H -1.79700100 1.96678700 -1.27281200 O -2.21369000 -1.13152000 -0.52205500 O -2.97671500 -0.33950200 0.26905300 C -2.47659200 -0.36920400 1.60673000 H -3.12611600 0.29424300 2.17708200 H -2.53077900 -1.38828400 1.99482100 H -1.44715000 -0.00574900 1.62448800
PC at NH in ethanol	0 2 C -0.91508600 -0.07368100 -0.11219700 C -1.44439900 1.22940600 -0.00442600 C -2.80573500 1.41095700 0.16092800 C -3.65883400 0.30637000 0.22162700 C -3.13772900 -0.98499700 0.11518500 C -1.77751300 -1.18836300 -0.05054400 H -0.76637100 2.07452200 -0.05281800 H -1.37524500 -2.18938300 -0.13336900 N 0.44345100 -0.15165200 -0.27254500 H 1.92200900 1.02587800 -0.64726800 O 0.86394300 -1.43263100 -0.36017000 H 1.83207100 -1.35374400 -0.44604900 O 2.89519600 1.12054100 -0.73606200 O 3.33331300 -0.14261800 -0.25395600

	C 3.61020700 -0.01233700 1.13652700 H 3.96136900 -0.99684100 1.44967500 H 4.39061000 0.73410100 1.29574800 H 2.70265500 0.25582400 1.68370200 H -4.72503000 0.45099200 0.35133900 H -3.20855400 2.41366700 0.24404600 H -3.80274600 -1.83990800 0.16171400
S3B2. ArNHOH + $CH_3COO^{\bullet}$ at the O-H bond in ethanol	
RC at OH in ethanol	0 2 C 0.28548400 -0.91584200 -0.28504200 C 0.55762700 -0.67552400 1.06187400 C 2.60554200 0.46594700 0.44868800 C 1.17625100 -0.46207900 -1.26604300 H -0.13069100 -1.01924100 1.82246000 H 0.95425900 -0.64439600 -2.31290600 N -0.90976900 -1.52358500 -0.72031700 H -0.74534600 -2.21465200 -1.44722800 O -1.61583000 -2.16810400 0.30831200 H -2.38166000 -1.59931900 0.46610100 O -2.21442800 0.83308100 0.65308400 O -1.81962500 1.37901000 -0.45090500 C -0.80654500 2.38472000 -0.23332900 H -1.24980500 3.20282500 0.33464800 H 0.02454300 1.93086500 0.30675100 H -0.50746200 2.71092400 -1.22726800 C 2.32562900 0.22173900 -0.89696800 C 1.71781300 0.01165700 1.41761800 H 1.92179500 0.19244700 2.46746800 H 3.50326900 1.00204000 0.73320000 H 3.00773200 0.56798200 -1.66573000
TS at OH in ethanol 1 imaginary frequencies ignored (-1286.1377 cm^{-1}) Distance (D): D(HN**O**....**H**)= 1.04162 Å D(**H**...**O**OCH_3)= 1.44188 Å Angle (∠) ∠(HN)**O-H-O**(OCH_3) = 159.571 °	0 2 C -0.69775400 0.11298300 0.51717700 C -1.48685500 1.26692200 0.41290400 C -2.74617100 1.18435100 -0.16040800 C -3.23087100 -0.03482000 -0.63688700 C -2.43838800 -1.17447500 -0.53111700 C -1.17229900 -1.11325800 0.04118500 H -1.10567200 2.21214900 0.78501300 H -3.35566900 2.07792100 -0.23412600 H -4.21637300 -0.09327100 -1.08327700 H -2.80643500 -2.12635900 -0.89723500 H -0.55790700 -2.00055900 0.12460700

	N 0.57913600 0.22889500 1.04671800 H 0.82128600 1.05136700 1.59045100 O 1.23558400 -0.88320400 1.42639700 H 1.83613600 -1.14629100 0.61701500 O 2.50079400 -1.05277400 -0.65911800 O 2.15471400 0.19627400 -0.98882500 C 3.12934400 1.13414800 -0.51455900 H 4.06074300 0.98040900 -1.06231700 H 2.71443800 2.11980700 -0.71980600 H 3.28472200 0.98508400 0.55524700
PC at OH in ethanol	0 2 C 0.99043000 -0.07081400 -0.10734400 C 1.79255900 -1.16331600 0.23125900 C 3.16453000 -0.97820800 0.33599100 C 3.73253700 0.27458200 0.10773400 C 2.91887400 1.35607100 -0.22938800 C 1.54602100 1.19161200 -0.33918700 H 1.34045700 -2.13138300 0.40493000 H 0.90117000 2.02413600 -0.60079500 N -0.39248500 -0.21316100 -0.22440600 H -0.96784600 0.59512800 -0.47969800 O -0.99579800 -1.31449700 -0.02500900 H -2.79000900 -1.17938300 -0.48857100 O -3.60992000 -0.66451500 -0.63618800 O -3.15904900 0.65103800 -0.34365200 C -3.36829100 0.88765400 1.04236900 H -4.42872900 0.79920300 1.28791100 H -2.77651600 0.19170100 1.64374100 H -3.02917300 1.91118500 1.21141700 H 3.35597200 2.33167700 -0.40731400 H 4.80458200 0.40797600 0.19210800 H 3.79566500 -1.81979500 0.59729600

Table S4. Rate constants of ArNHOH + $CH_3OO^{\bullet}$ reactions in the gas phase

Temperature in Kelvin (K)	Rate constants in cm^3/molecule/s	
	$k_{O\text{-}H}$	$k_{N\text{-}H}$
283	1.60E-14	4.50E-15
293	1.40E-14	3.80E-15
298.15	1.30E-14	3.50E-15
303	1.30E-14	3.30E-15
313	1.20E-14	2.90E-15
323	1.10E-14	2.60E-15
333	1.10E-14	2.40E-15
343	1.00E-14	2.30E-15
353	9.90E-15	2.20E-15
363	9.60E-15	2.10E-15
373	9.40E-15	2.00E-15
383	9.30E-15	2.00E-15
393	9.20E-15	2.00E-15
403	9.10E-15	2.00E-15
413	9.10E-15	2.00E-15
423	9.10E-15	2.00E-15
433	9.10E-15	2.00E-15
443	9.10E-15	2.10E-15
453	9.20E-15	2.10E-15
463	9.30E-15	2.20E-15
473	9.40E-15	2.20E-15
483	9.50E-15	2.30E-15
493	9.70E-15	2.40E-15
503	9.80E-15	2.50E-15
513	1.00E-14	2.50E-15
523	1.00E-14	2.60E-15
533	1.00E-14	2.70E-15
543	1.10E-14	2.90E-15
553	1.10E-14	3.00E-15
563	1.10E-14	3.10E-15
573	1.10E-14	3.20E-15
583	1.10E-14	3.40E-15
593	1.20E-14	3.50E-15
603	1.20E-14	3.60E-15

613	1.20E-14	3.80E-15
623	1.30E-14	4.00E-15
633	1.30E-14	4.10E-15
643	1.30E-14	4.30E-15
653	1.30E-14	4.50E-15
663	1.40E-14	4.70E-15
673	1.40E-14	4.90E-15
683	1.40E-14	5.10E-15
693	1.50E-14	5.30E-15
703	1.50E-14	5.60E-15
713	1.60E-14	5.80E-15
723	1.60E-14	6.00E-15
733	1.60E-14	6.30E-15
743	1.70E-14	6.60E-15
753	1.70E-14	6.80E-15
763	1.80E-14	7.10E-15
773	1.80E-14	7.40E-15
783	1.90E-14	7.70E-15
793	1.90E-14	8.00E-15
803	1.90E-14	8.40E-15
813	2.00E-14	8.70E-15
823	2.00E-14	9.10E-15
833	2.10E-14	9.40E-15
843	2.20E-14	9.80E-15
853	2.20E-14	1.00E-14
863	2.30E-14	1.10E-14
873	2.30E-14	1.10E-14

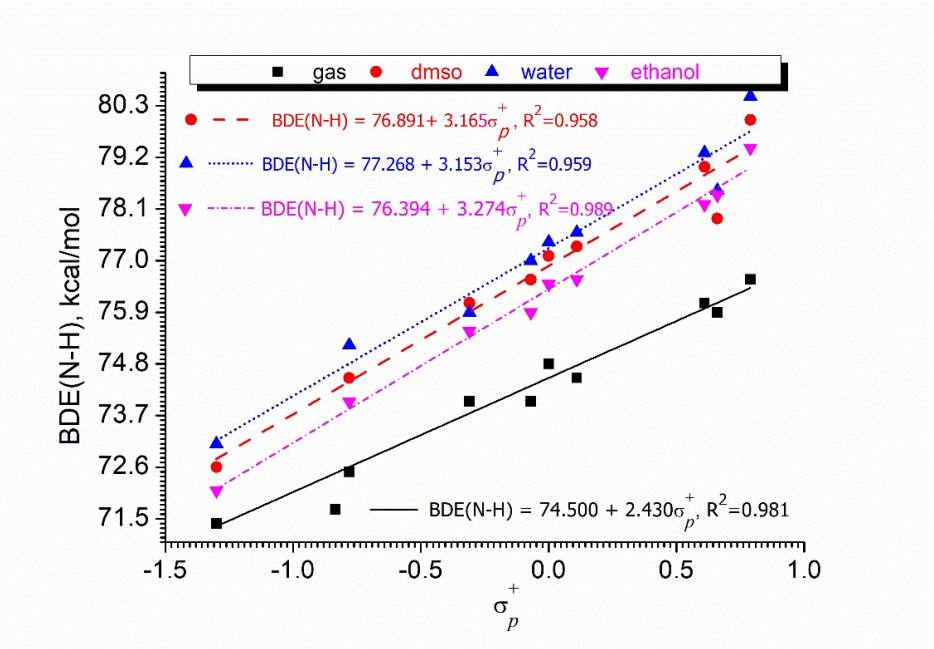
Table S5. Gibbs free energies in kcal/mol for ArNHOH + $CH_3OO^{\bullet}$ reactions in the gas phase

Temperature in Kelvin (K)	O-H	N-H
0	-14	-9
283	-13.9	-8.9
293	-13.9	-8.9
298.15	-13.9	-8.9
303	-13.9	-8.9
313	-13.9	-8.9
323	-13.9	-8.9
333	-13.9	-8.9
343	-13.9	-8.9
353	-13.9	-8.9
363	-14	-8.9
373	-14	-8.9
383	-14	-8.9
393	-14	-8.9
403	-14	-8.9
413	-14	-8.9
423	-14	-8.9
433	-14	-8.9
443	-14	-8.9
453	-14	-8.9
463	-14	-8.9
473	-14	-8.9
483	-14	-9
493	-14	-9
503	-14	-9
513	-14	-9
523	-14	-9
533	-14	-9
543	-14	-9

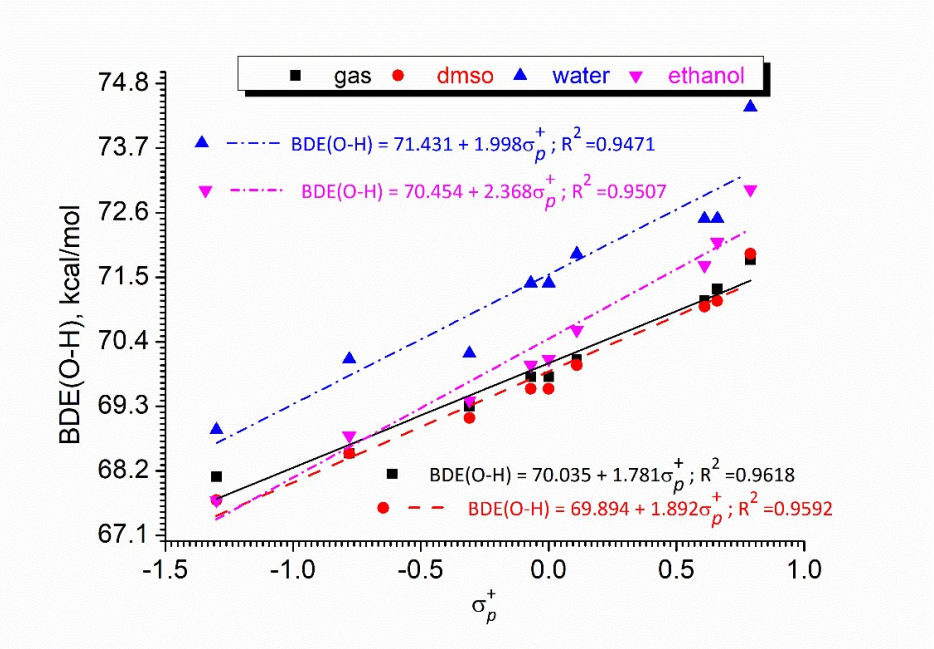
553	-14	-9
563	-14.1	-9
573	-14.1	-9
583	-14.1	-9
593	-14.1	-9
603	-14.1	-9
613	-14.1	-9
623	-14.1	-9
633	-14.1	-9.1
643	-14.1	-9.1
653	-14.1	-9.1
663	-14.1	-9.1
673	-14.1	-9.1
683	-14.1	-9.1
693	-14.1	-9.1
703	-14.1	-9.1
713	-14.1	-9.1
723	-14.1	-9.1
733	-14.1	-9.1
743	-14.2	-9.1
753	-14.2	-9.2
763	-14.2	-9.2
773	-14.2	-9.2
783	-14.2	-9.2
793	-14.2	-9.2
803	-14.2	-9.2
813	-14.2	-9.2
823	-14.2	-9.2
833	-14.2	-9.2
843	-14.2	-9.2
853	-14.2	-9.2
863	-14.2	-9.3
873	-14.2	-9.3

Table S6. Gibbs free energies in kcal/mol for ArNHOH + $CH_3OO^{\bullet}$ reactions in ethanol

Temperature in Kelvin (K)	O-H	N-H
0	-16.0	-9.6
298.15	-15.9	-9.5



a) BDE(N-H) vs σ_p^+



b) BDE(O-H) vs σ_p^+

Fig. S1 Correlations between calculated a) BDE(N–H) and b) BDE(O-H) with σ_p^+ constant in four media

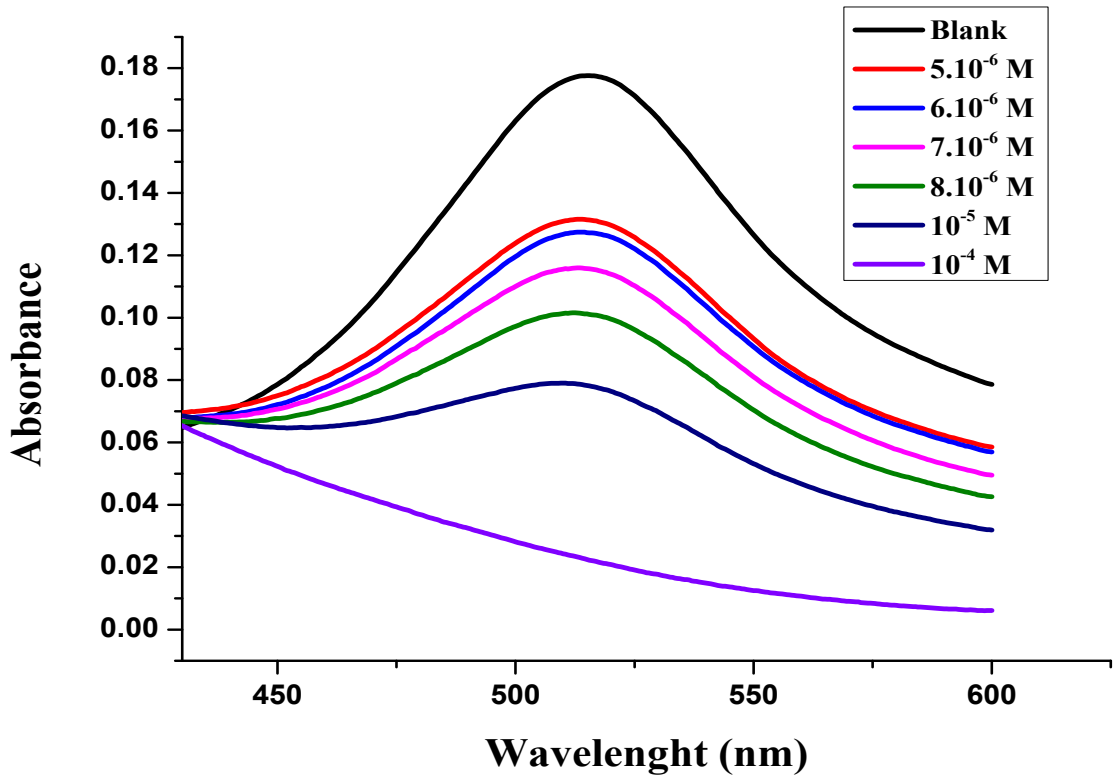


Fig. S2 UV-VIS spectra of DPPH• with various concentrations of ArNHOH