Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
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Hydroxyl Radical Formation in the Gas Phase Oxidation of Distonic 2-Methylphenyl Radical Cations

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SUPPORTING INFORMATION

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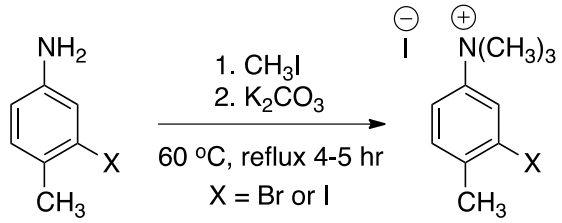
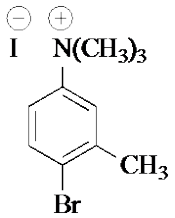
1. Methylation of halogen-substituted methylaniline



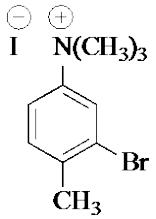
Scheme S1 Overview of synthesis for *N*,*N*,*N*-trimethylammonium charge tagged aniline derivatives

The 4-iodomethyl-*N*,*N*,*N*-trimethylbenzenaminium, 3-iodo-*N*,*N*,*N*,4-tetramethylbenzenaminium, 3-bromo-*N*,*N*,*N*,4-tetramethylbenzenaminium and 4-bromo-*N*,*N*,*N*,3-tetramethylbenzenaminium iodide salts were synthesised using a modified procedure previously reported by Kirk *et. al.* for the synthesis of 4-iodo-*N*,*N*,*N*,-trimethylbenzenaminium iodide.[1] In brief, to a reaction vial was added halogenated aniline species (*ca.* 1 mmol), 10 mL of dry CH_3OH, and CH_3I (0.7 mL, 10 mol equiv) that was then heated at reflux for two hours. K_2CO_3 (0.2 g, 1.3 mmol) was added to the reaction vial and the solution heated at reflux for a further two hours. The solvent was removed *in vacuo* and the crude product recrystallised from CH_3CN. The recrystallised solid was washed with diethyl ether and dried.

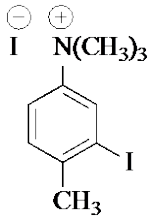
2. Structural characterisation



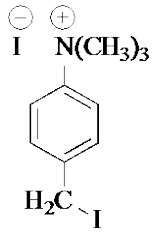
4-bromo-3-methyl-N,N,N-trimethylbenzenaminium iodide. ^{1}H NMR (300 MHz, D_2O): δ 2.49 (s, 3H), δ 3.64 (s, 9H), δ 7.55 (dd, 1H, *J* = 8.79, 3.21 Hz), δ 7.80 (d, 1H, *J* = 2.05 Hz), δ7.21 (d, 1H, *J* = 9.07 Hz).



3-bromo-4-methyl-N,N,N-trimethylbenzenaminium iodide. ^{1}H NMR (300 MHz, D_2O): δ 2.45 (s, 3H), δ 3.64 (s, 9H), δ 7.55 (d, 1H, *J* = 8.79 Hz), δ 7.72 (dd, 1H, *J* = 8.5, 2.64 Hz), δ 8.10 (d, 1H, *J* = 2.93 Hz).



3-iodo-4-methyl-N,N,N-trimethylbenzenaminium iodide. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.35 (s, 1H), δ 7.90 (d, H, *J* = 7.3 Hz), δ 7.56 (d, 1H, *J* = 8.8 Hz), δ 3.57 (s, 9H), δ 2.43 (s, 3H).



3-iodo-4-methyl-N,N,N-trimethylbenzenaminium iodide. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.90 (d, 2H, J = 8.6 Hz), δ 7.67 (d, 2H, J = 8.8 Hz), δ 4.67 (s, 2H), δ 3.59 (s, 9H).

3. Supplementary Mass Spectra

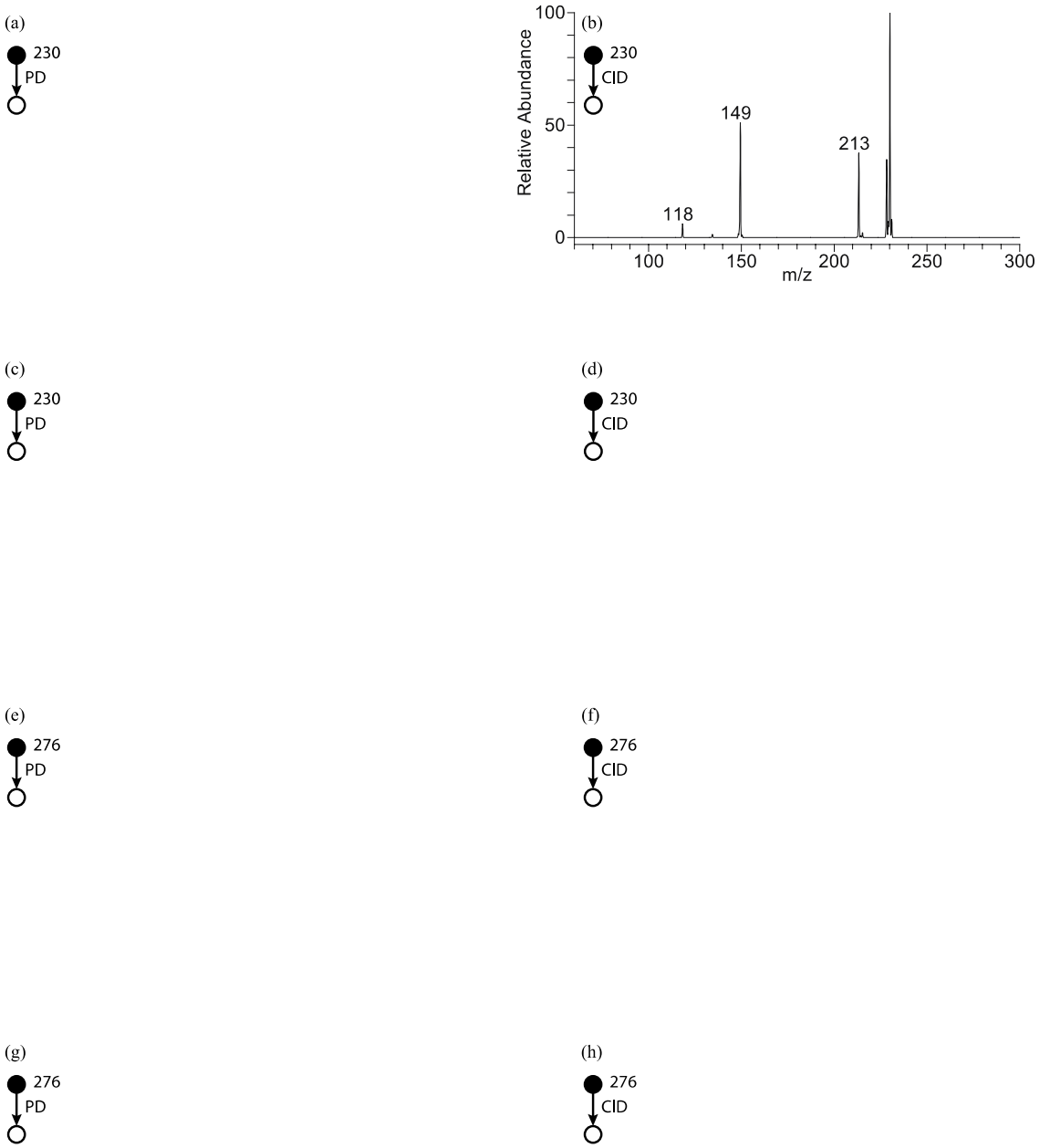


Figure S1 Gas-phase ions produced by ESI of 4Br3Me (a and b), 3Br4Me (c and d), 3I4Me (e and f) and 4IMe (g and h) were isolated and activated by PD (left panel) and CID (right panel) to generate the *m/z* 149 ions via loss of the halogen

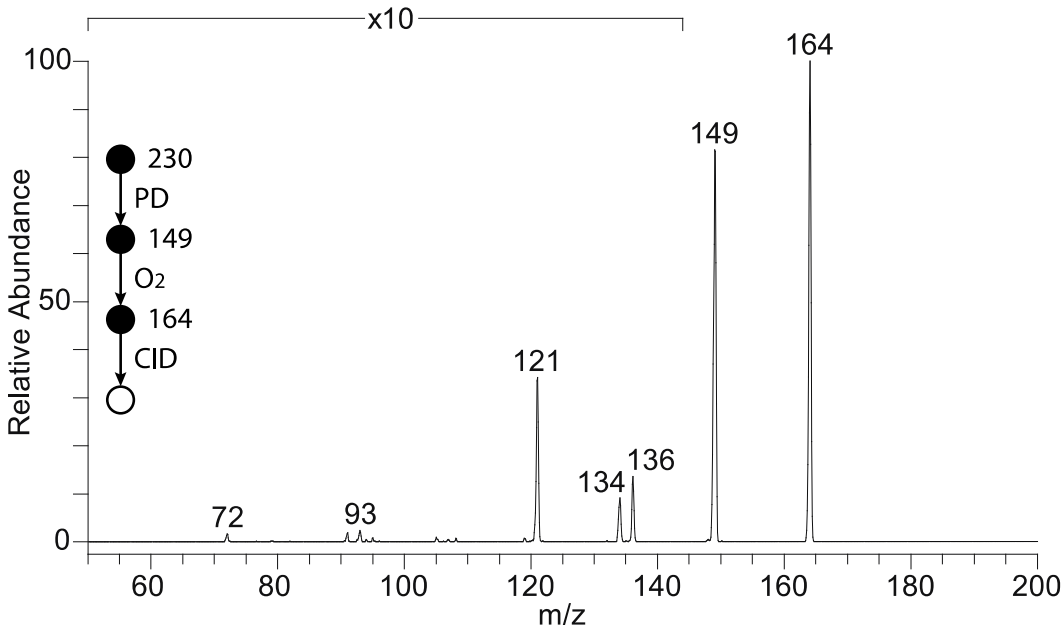


Figure S2 CID of *m/z* 164 ions generated via PD of 3-bromo-4,N,N,N-tetramethylbenzenaminium (3Br4Me) and subsequent isolation of the resultant *m/z* 149 ions for 10 s in the presence of background O_2. Peaks at *m/z* 149 (15 Da loss), 136 (28 Da loss), and 121 (43 Da loss) are consistent with loss of CH_3, CO, and both CH_3 and CO, respectively.[2, 3]

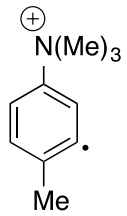
4. Computational results

Table S1 Comparison of M06-2X/6-311++G(d,p) and G3SX(MP3) energies presented in kcal mol^{-1} relative to the initial intermediate (II) for the charge-tagged 2-methylphenyl + O_2 reaction.

Structure	M06-2X/6-311++G(d,p) (kcal mol^{-1})	G3SX(MP3) (kcal mol^{-1})	Difference (kcal mol^{-1})
I	42.96	46.37	3.41
II	0.00	0.00	0.00
III	37.52	38.83	1.31
TS II→IV	28.86	25.38	3.48
IV	19.50	16.02	3.48
TS1	44.00	37.51	6.49
TS2	37.77	30.65	7.12
V	-41.66	-42.40	0.74
VI	-46.50	-47.02	0.52
TS II→VII	28.65	27.23	1.42
VII	4.72	4.51	0.21
TS VII→VIII	14.88	13.91	0.97
VIII	1.46	-3.96	5.42
		Average difference	2.7

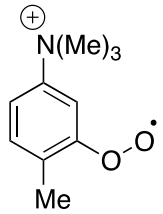
Table S2 Geometries optimised by M06-2X/6-311++G(d,p) method provided in Cartesian coordinates for intermediates and transition states identified in Figure 3 of the main document

I (1, 2)			
C	0.32731600	0.00701000	0.00029700
C	-0.33414800	-1.22630700	-0.00172300
C	-1.69962000	-1.17968600	-0.00301500
C	-2.49685700	-0.05212700	-0.00311800
C	-1.79055800	1.15201600	-0.00274400
C	-0.39473700	1.19119100	-0.00031400
H	-2.33851800	2.08809900	-0.00565200
H	0.08548900	2.15855200	-0.00047700
C	-3.99790100	-0.11714400	0.00335300
H	-4.35657700	-0.77128400	-0.79229700
H	-4.35409800	-0.52365900	0.95212900
H	-4.43108500	0.87298900	-0.13322200
H	0.18459800	-2.17838500	-0.00319300
N	1.82779200	0.00130200	0.00066100
C	2.32867400	-0.70232600	-1.23195200
C	2.32829000	-0.71124500	1.22834100
C	2.41011600	1.38208600	0.00597900
H	3.41757800	-0.67311800	-1.22589800
H	1.98249300	-1.73214700	-1.22253500
H	1.93282100	-0.18399900	-2.10341700
H	3.41716700	-0.68124200	1.22319500



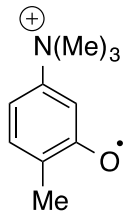
H	1.93149800	-0.19976400	2.10339400
H	1.98297600	-1.74123400	1.21101800
H	2.08850000	1.91002700	-0.88912900
H	2.08554300	1.90408900	0.90353100
H	3.49361000	1.28114600	0.00730900

II
(1, 2)



C	-1.94897200	-0.97658300	0.00000000
C	-0.93775400	-1.93580400	-0.00000300
C	0.40630800	-1.58696200	0.00000500
C	0.76226300	-0.24231000	0.00002100
C	-0.20406700	0.75019000	0.00001700
C	-1.53284600	0.35204700	0.00000600
H	-1.20955400	-2.98485100	-0.00001400
H	1.14859500	-2.37503100	-0.00001200
H	0.00276800	1.80913900	0.00002900
C	-3.40709300	-1.33209200	0.00000500
H	-3.90439200	-0.91620200	-0.87844600
H	-3.53751100	-2.41283600	-0.00010600
H	-3.90433000	-0.91639500	0.87858400
O	-2.56275600	1.28852000	0.00000900
O	-2.17819500	2.52930800	-0.00002200
N	2.21977700	0.10910700	0.00000100
C	2.87556500	-0.45820300	1.23083700
H	2.77944000	-1.54039100	1.22319000
H	3.92740500	-0.17506500	1.21941400
H	2.37427600	-0.04450000	2.10405600
C	2.45550900	1.59014800	-0.00007600
H	2.01665500	2.02305000	-0.89652600
H	2.01654100	2.02315700	0.89626700
H	3.53158600	1.75149000	-0.00002400
C	2.87553500	-0.45834300	-1.23078600
H	3.92740200	-0.17530600	-1.21936900
H	2.77929000	-1.54052100	-1.22306400
H	2.37429700	-0.04464800	-2.10403900

III
(1, 2)



C	2.25488200	-0.45601600	-0.00002900
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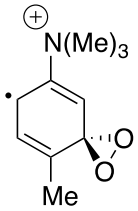
C	0.00724800	-1.37216000	-0.00011500
C	-0.55806300	-0.07454900	-0.00001100

C	0.23542300	1.03111700	0.00008100
C	1.68691300	0.88847600	0.00007400
H	1.79036300	-2.54421000	-0.00020400
H	-0.61787000	-2.25641500	-0.00019600
H	-0.12171300	2.05134600	0.00016500
C	3.73605000	-0.59109600	-0.00003800
H	4.15769500	-0.08612400	0.87307500
H	4.04241900	-1.63573600	-0.00005000
H	4.15767900	-0.08611800	-0.87315600
O	2.40270100	1.89480900	0.00015600
N	-2.05379800	0.03370700	-0.00000100
C	-2.60734000	-0.63163000	-1.23189700
H	-2.34833600	-1.68694400	-1.22057400
H	-3.69007300	-0.51383600	-1.22644600
H	-2.17135000	-0.14789500	-2.10423900
C	-2.52156800	1.45885700	-0.00003300
H	-2.15570400	1.95530700	0.89618600
H	-2.15577100	1.95524500	-0.89631300
H	-3.60966700	1.44737200	0.00001100
C	-2.60731800	-0.63156800	1.23193700
H	-3.69004700	-0.51373300	1.22652000
H	-2.34834800	-1.68689000	1.22064800
H	-2.17128000	-0.14781700	2.10424800

TS II→IV (1, 2)			
C	0.77450600	0.24509600	0.03696700
C	-0.11338200	-0.79106800	0.23538600
C	-1.49697700	-0.51246700	0.23357200
C	-1.99781600	0.81109500	0.07804100
C	-1.06111100	1.81213700	-0.10970600
C	0.31170500	1.55051500	-0.13690300
H	-1.39726000	2.83408000	-0.23741200
H	0.98516700	2.38065000	-0.29190200
C	-3.47114100	1.04010700	0.10809700
H	-3.95797600	0.39219200	-0.62497300
H	-3.87525100	0.77063400	1.08734900
H	-3.71155500	2.07996900	-0.10523900
O	-2.35458000	-1.53414500	0.53829900
O	-2.26227700	-1.61926600	-0.88214300
H	0.17011400	-1.82618900	0.37887300
N	2.23754700	-0.08014500	0.00614100
C	2.51364200	-1.03365300	-1.12751900
C	2.64627800	-0.71297700	1.31002300

C	3.09297100	1.13385200	-0.19874600
H	3.58337500	-1.23745100	-1.15024800
H	1.95972000	-1.95424300	-0.96465600
H	2.18927500	-0.56302000	-2.05396200
H	3.71549100	-0.91650400	1.27002000
H	2.41603800	-0.01628100	2.11413000
H	2.09636700	-1.63972400	1.44917700
H	2.84702000	1.58931900	-1.15574100
H	2.92847300	1.83173400	0.61957900
H	4.13098800	0.80729700	-0.20249700

IV
(1, 2)



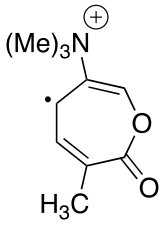
C	-2.01100800	0.79616000	-0.00019500
C	-1.05717800	1.78401800	-0.00099400
C	0.31581000	1.50429700	-0.00103800
C	0.76638700	0.15605900	-0.00014400
C	-0.10431900	-0.87944400	0.00039800
C	-1.55361500	-0.61042900	-0.00014100
H	-1.37255600	2.82080200	-0.00138400
H	1.01386700	2.33035900	-0.00160400
H	0.15855900	-1.92742900	0.00096900
C	-3.47793400	1.04389800	0.00139300
H	-3.93608600	0.58367400	0.88142100
H	-3.69685900	2.10998300	-0.00418800
H	-3.94033700	0.57311800	-0.87068300
O	-2.31661800	-1.52955600	0.72721800
O	-2.31575300	-1.52948300	-0.72863200
N	2.24653800	-0.07728200	0.00021800
C	2.85213900	0.54051700	-1.23229500
H	2.67498700	1.61237900	-1.22482000
H	3.92229900	0.33879600	-1.22340500
H	2.38216900	0.08908400	-2.10431600
C	2.59778700	-1.53538300	0.00114300
H	2.19333000	-2.00018900	0.89785800
H	2.19363100	-2.00125800	-0.89515100
H	3.68330500	-1.61183800	0.00137800
C	2.85174700	0.54199100	1.23218400
H	2.38160500	0.09150300	2.10460000
H	3.92193200	0.34038400	1.22380500
H	2.67446800	1.61382300	1.22344300

TS1 (1, 2)			
C	-2.04038400	0.74057500	-0.02673900
C	-1.10270600	1.74668500	0.02939800
C	0.26922600	1.48711800	0.03176100
C	0.74742300	0.14875500	-0.02257400
C	-0.10434000	-0.89946300	-0.07518200
C	-1.58230300	-0.68680500	-0.02845900
H	-1.43471300	2.77769500	0.06628900
H	0.95340000	2.32407200	0.08021200
H	0.18214000	-1.94121000	-0.10966800
N	2.23306600	-0.05497700	-0.01102500
O	-2.11881700	-1.40307200	1.03494400
O	-2.28808000	-1.52996400	-0.86974200
C	2.80579200	0.51041900	1.26171300
H	3.87898400	0.32535900	1.26419000
H	2.61249300	1.57890700	1.30272100
H	2.32627900	0.01005100	2.10132700
C	2.84699700	0.63622200	-1.19910100
H	3.92116000	0.45777500	-1.17966200
H	2.40386000	0.21958300	-2.10191500
H	2.64706800	1.70267800	-1.14218900
C	2.61146700	-1.50487000	-0.07829200
H	2.20424300	-2.02140700	0.78832300
H	2.22705100	-1.93198000	-1.00222300
H	3.69813200	-1.56171200	-0.06713800
C	-3.50721200	0.96955300	-0.06087300
H	-4.00198400	0.32487400	0.67076500
H	-3.75409600	2.01144400	0.13514700
H	-3.90405900	0.68385600	-1.04052800

TS2 (1, 2)			
C	-2.07926100	0.66755600	-0.11121300
C	-1.15385300	1.71643100	-0.06460500
C	0.19705600	1.45760000	-0.10652200
C	0.72363300	0.13791800	-0.16912000
C	-0.12262800	-0.91877800	-0.24807800
C	-1.59554500	-0.74336900	-0.11633300
H	-1.50090800	2.73843400	0.02123200
H	0.86954900	2.30656000	-0.03538800
H	0.16983800	-1.96025700	-0.26114700
N	2.20237800	-0.03544700	-0.01307000
O	-1.69446700	-1.04138900	1.22760100

O	-2.36376000	-1.66041300	-0.74898300
C	2.62187000	0.47329500	1.34212500
H	3.68904700	0.29213000	1.46280200
H	2.41769300	1.53957800	1.40447800
H	2.04857100	-0.06318500	2.09655100
C	2.93154100	0.71584800	-1.09256000
H	4.00086700	0.56550100	-0.95211700
H	2.61146700	0.32481400	-2.05659600
H	2.69950200	1.77522400	-1.02142000
C	2.60750500	-1.47778200	-0.10466900
H	2.14388500	-2.03188000	0.70867600
H	2.30106600	-1.87360100	-1.07103400
H	3.69071500	-1.52064000	-0.01157100
C	-3.52870200	0.84703400	-0.00836900
H	-3.87452500	0.17147500	0.78726600
H	-3.82425800	1.87429700	0.18917900
H	-4.00303900	0.46958000	-0.92230500

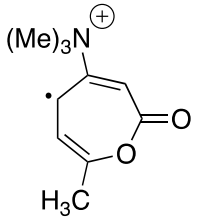
V
(1, 2)



C	0.81213200	0.01151700	-0.15430900
C	0.22334100	1.22425300	-0.27729500
C	-2.17788800	0.81876600	0.02241800
C	-2.27475900	-0.64653400	-0.02838800
C	-1.21070000	-1.49981000	-0.24843900
C	0.15875600	-1.25048600	-0.29149500
H	0.77864000	-2.12899400	-0.41357500
O	-1.05646200	1.44247800	-0.58887200
O	-3.02138800	1.54042300	0.43145300
C	-3.66007400	-1.16505700	0.19527900
H	-4.35795800	-0.72313400	-0.52078100
H	-3.69203200	-2.24957900	0.10777500
H	-4.01319000	-0.87472500	1.18862500
H	-1.47679000	-2.54832000	-0.33986200
H	0.76753900	2.15597800	-0.21332300
N	2.29271800	-0.04534900	0.10193400
C	2.55724700	-0.84795800	1.34982100
H	3.63326300	-0.87782900	1.51452000
H	2.05313500	-0.35680000	2.18031600
H	2.16989700	-1.85459200	1.22322700
C	2.98685200	-0.68593400	-1.07289600
H	2.75096400	-0.10534400	-1.96285300
H	4.05853100	-0.67894400	-0.87945800
H	2.64099100	-1.70849300	-1.19080100

C	2.92123900	1.30355700	0.30407000
H	2.44399700	1.80156100	1.14550300
H	3.97476600	1.14068200	0.52163200
H	2.82514200	1.88888100	-0.60772800

VI
(1, 2)



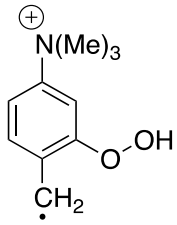
C	1.29544400	-1.59819500	0.00004800
C	2.36337400	-0.73968900	-0.00004600
C	1.30511400	1.51889700	-0.00000500
C	-0.11745400	1.14232600	-0.00034300
C	-0.70626300	-0.08793200	-0.00005200
C	-0.08428500	-1.34564900	0.00014400
H	1.57729200	-2.64340000	0.00002200
H	-0.70070800	2.04813100	-0.00059800
H	-0.70379400	-2.23160200	0.00026700
O	2.34497200	0.60579500	0.00017700
O	1.62024600	2.66492800	0.00010800
C	3.77412900	-1.21631500	-0.00015400
H	4.28929400	-0.82155800	0.87928900
H	3.83049600	-2.30207400	-0.00077100
H	4.28948100	-0.82052700	-0.87902100
N	-2.22323200	-0.13675500	-0.00002200
C	-2.70326800	-0.85487000	-1.23502400
H	-2.35088200	-1.88151300	-1.22522600
H	-3.79215000	-0.83606700	-1.23606800
H	-2.30938300	-0.33181700	-2.10493200
C	-2.70307900	-0.85406800	1.23553800
H	-2.30911000	-0.33038900	2.10503500
H	-3.79196100	-0.83533500	1.23670200
H	-2.35058400	-1.88068100	1.22638200
C	-2.87559700	1.21651400	-0.00039700
H	-2.58729800	1.75948500	0.89676700
H	-2.58735100	1.75896200	-0.89789600
H	-3.95114700	1.05376800	-0.00033700

TS II→VII
(1, 2)

C	0.87803200	0.21635300	0.00896500
C	-0.05438900	-0.81257200	0.08328300
C	-1.39928500	-0.48370000	0.10119700
C	-1.84904600	0.84258700	0.04532500
C	-0.88585800	1.83873900	-0.03317000

C	0.47788400	1.54188100	-0.05600700
H	-1.19704800	2.87602800	-0.07219200
H	1.17917000	2.35965700	-0.12328500
C	-3.31465800	1.09990600	0.11702800
H	-3.75085600	-0.14753700	-0.06502400
H	-3.69322400	1.42463400	1.08490600
H	-3.75523200	1.61117400	-0.73617400
O	-2.28985500	-1.49863200	0.27945800
O	-3.47280300	-1.25242000	-0.41253600
H	0.20685000	-1.86246100	0.12305800
N	2.32853700	-0.16402700	-0.01479200
C	2.60508800	-1.02691800	-1.21771300
C	2.67320300	-0.92013500	1.24085500
C	3.23319100	1.02861900	-0.09243800
H	3.66713700	-1.26873000	-1.22844400
H	2.01534000	-1.93699700	-1.15166300
H	2.32728600	-0.46646200	-2.10854000
H	3.73513300	-1.16085000	1.21444700
H	2.44176900	-0.28515200	2.09415600
H	2.08422400	-1.83209100	1.28447300
H	3.02763800	1.57423700	-1.01086600
H	3.06989700	1.65834200	0.77954800
H	4.25844900	0.66425000	-0.10018400

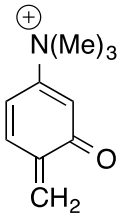
VII
(1, 2)



C	1.87048400	0.98334400	0.08588100
C	0.84174300	1.93161600	-0.12261500
C	-0.49546200	1.57845900	-0.15849900
C	-0.85475900	0.24217000	0.00614100
C	0.12540900	-0.73503600	0.19033200
C	1.45309300	-0.36918600	0.23437900
H	1.11286700	2.97366900	-0.24257300
H	-1.22568000	2.35973400	-0.31024000
H	-0.09786800	-1.78815900	0.30673000
C	3.21891100	1.36095900	0.17228900
H	3.76192500	-2.21147600	-0.40130200
H	3.49780500	2.40070100	0.06961900
H	3.99208800	0.62791300	0.34328400
O	2.35735700	-1.35883300	0.49342200
O	3.18733400	-1.48585000	-0.68336700
N	-2.28512500	-0.19990400	-0.01532700
C	-3.23196800	0.93685900	-0.25339000
H	-3.01539900	1.38648400	-1.22019000

H	-4.24188300	0.53130300	-0.25141200
H	-3.12527200	1.66584100	0.54691600
C	-2.64103300	-0.82353300	1.30773600
H	-2.00403800	-1.68706200	1.47979900
H	-2.47920300	-0.08077700	2.08678300
H	-3.68662400	-1.12789000	1.27483100
C	-2.49159400	-1.20404000	-1.11809600
H	-3.54427300	-1.48386600	-1.13512700
H	-2.19851500	-0.74019800	-2.05814500
H	-1.87653200	-2.07910000	-0.92707300

TS VII→VIII (1, 2)			
C	0.84086800	0.22897900	0.02390900
C	-0.11244900	-0.72344100	0.25234200
C	-1.48026600	-0.35322400	0.36177300
C	-1.86668800	1.02094700	0.12093300
C	-0.81816000	1.96837300	-0.11423700
C	0.49420100	1.59863700	-0.15564100
H	-1.08277500	3.00815600	-0.26814900
H	1.24041700	2.35835400	-0.33240900
C	-3.19396500	1.37037400	0.08878700
H	-3.68520100	-2.35826300	-0.45190400
H	-3.95796700	0.62028400	0.24413000
H	-3.49343700	2.39218800	-0.10894300
O	-2.34691400	-1.24985000	0.65756800
O	-3.19729100	-1.60749700	-0.82394900
H	0.10562400	-1.77544300	0.38925300
N	2.27608900	-0.21306200	-0.03195900
C	2.44500600	-1.24647200	-1.11504100
C	2.67319100	-0.80268000	1.29565900
C	3.21841300	0.91448600	-0.33018700
H	3.49705300	-1.52551500	-1.15862200
H	1.83747400	-2.11605500	-0.88096200
H	2.12118700	-0.80809500	-2.05732600
H	3.72154300	-1.09399200	1.24094700
H	2.52339700	-0.04504000	2.06283900
H	2.05234200	-1.66993000	1.50343200
H	2.96551900	1.34708700	-1.29591600
H	3.14987500	1.65840800	0.46051500
H	4.22505600	0.50219200	-0.36190000



VIII (1, 1)			
C	-2.32461500	0.47418500	-0.00004300
C	-1.42106600	1.60825300	-0.00000400
C	-0.08072600	1.46510700	-0.00000500
C	0.48784800	0.12772800	-0.00008800
C	-0.26377700	-0.98372300	-0.00016500
C	-1.74356800	-0.90386800	-0.00004700
H	-1.85209900	2.60346100	0.00001500
H	0.54250400	2.34524300	0.00000000
H	0.13550800	-1.99047400	-0.00021900
C	-3.66036500	0.62011900	-0.00003500
H	-4.12201800	1.60134200	0.00006300
H	-4.30096200	-0.25521000	0.00005000
O	-2.41166100	-1.90997300	0.00010600
N	1.98839300	-0.04116300	-0.00000200
C	2.72764100	1.26466700	-0.00013500
H	2.47139200	1.82461900	0.89657800
H	3.79198000	1.03770300	-0.00011400
H	2.47139800	1.82443600	-0.89696500
C	2.40681700	-0.80143700	-1.23147100
H	1.95402900	-1.78867200	-1.21527800
H	2.06762100	-0.24861100	-2.10592100
H	3.49283300	-0.88479600	-1.22607800
C	2.40659800	-0.80108900	1.23177400
H	3.49262100	-0.88436400	1.22665800
H	2.06714200	-0.24805900	2.10599400
H	1.95386000	-1.78835300	1.21570200

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3. G. da Silva and J. W. Bozzelli, Quantum Chemical Study of the Thermal Decomposition of O-Quinone Methide (6-Methylene-2,4-Cyclohexadien-1-One), *J. Phys. Chem. A*, 2007, **111**, 7987-7994.