

Supporting information: Early-stage oxidation and subsequent damage of the used nuclear fuel extractant TODGA; electron pulse radiolysis and theoretical insights

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NOTE: Supporting Information is broken into 4 sections referenced by the main manuscript:

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- 4) Optimized geometries (XYZ) determined by computations.....Page 13

1) Figures S1-S11

Fig. S1. Pulse radiolysis of 200 mM TODGA without (blue) and with (green) oxygen purging at 375 nm **(a)** and 600 nm **(b)**.

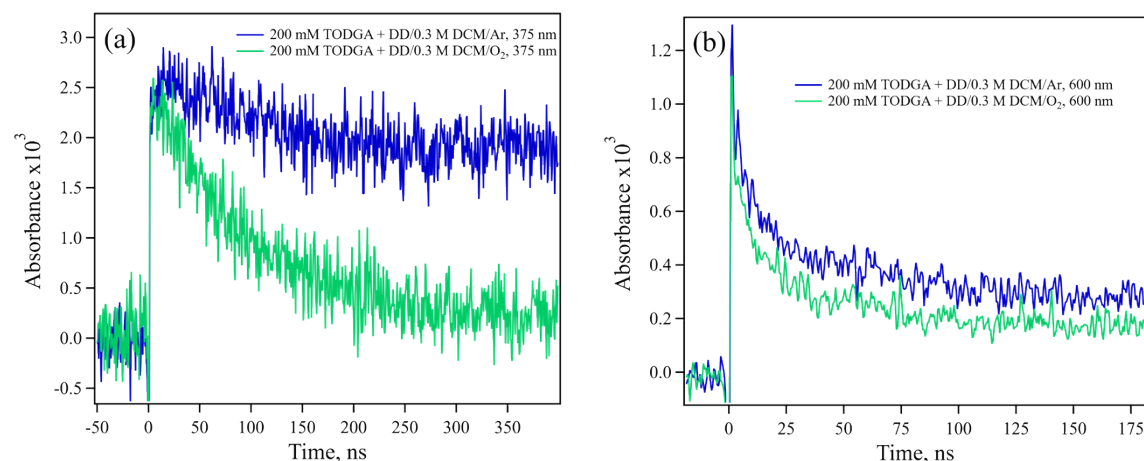


Fig. S2. Transient spectrum obtained for electron pulse-irradiated, 20 mM TODGA in DD/0.3 M DCM.

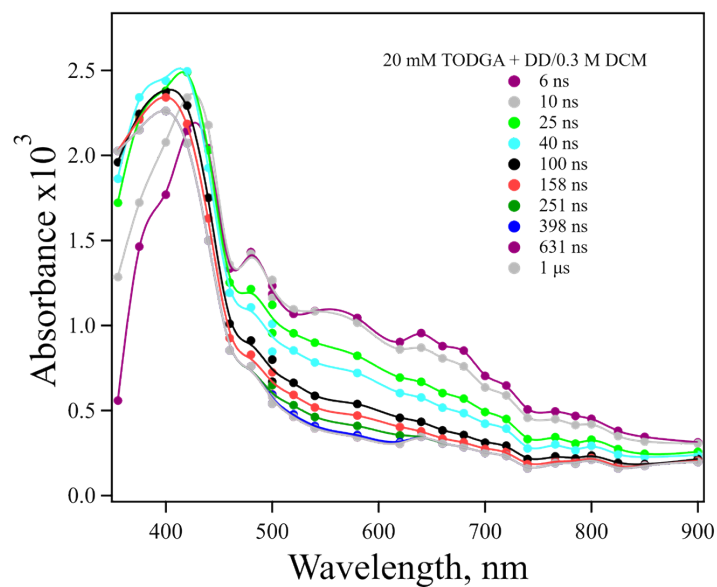


Fig. S3. Transient spectra obtained for electron pulse-irradiated, aerated DD/0.3 M DCM. Peak at 850 nm identified as $\text{DD}^{\bullet+}$.

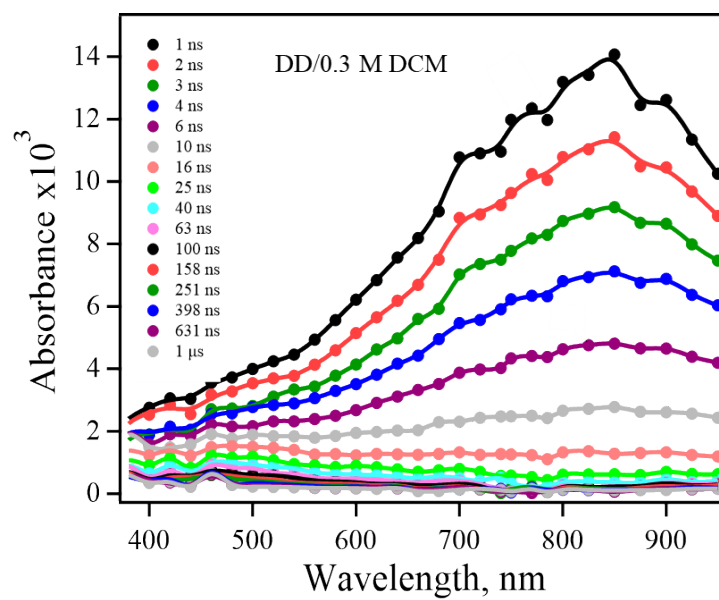


Fig. S4. Determination of rate constants for reaction of $\text{DD}^{\bullet+}$ with *p*-xylene (a) and TODGA (b) in DD/0.3 M DCM at 800 nm and 295 K. Rates were determined by the first exponential of biexponential fits over to raw kinetic data from 30 to 4000 ps. Solid line is weighted linear fit, corresponding to a slope of $(2.55 \pm 0.34) \times 10^{10} \text{ M}^{-1}\text{s}^{-1}$ for *p*-xylene and $(2.38 \pm 0.15) \times 10^{10} \text{ M}^{-1}\text{s}^{-1}$ for TODGA.

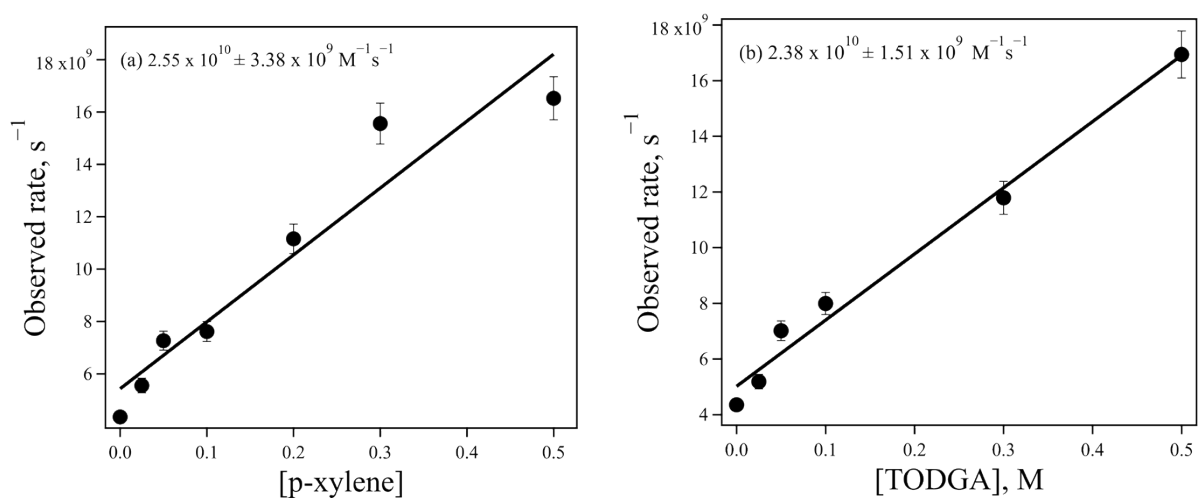


Fig. S5. Transient spectra obtained for electron pulse-irradiated, 50 mM TTA in DD/0.3 M DCM. Peak at 670 nm identified as $\text{TTA}^{\bullet+}$.

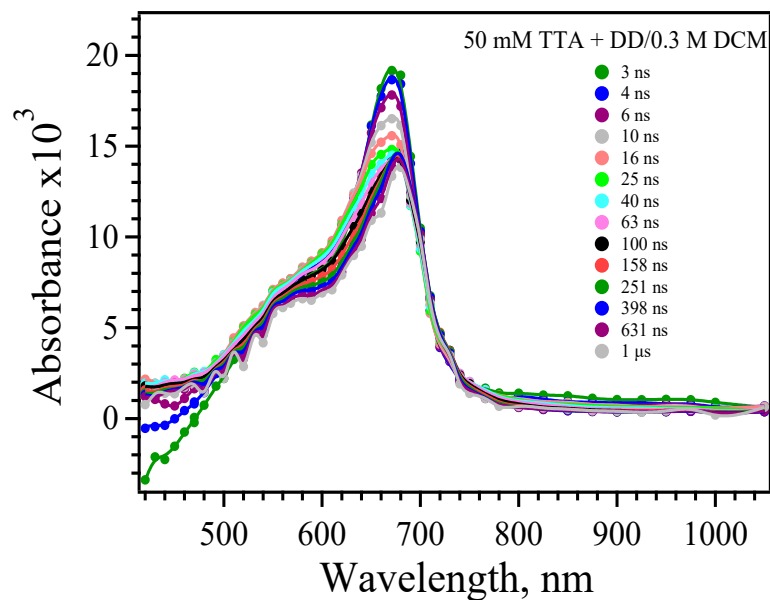


Fig. S6. Transient spectra obtained for electron pulse-irradiated, 2 mM TTA with 200 mM TODGA (a) and *p*-xylene (b) in DD/0.3 M DCM/ethene.

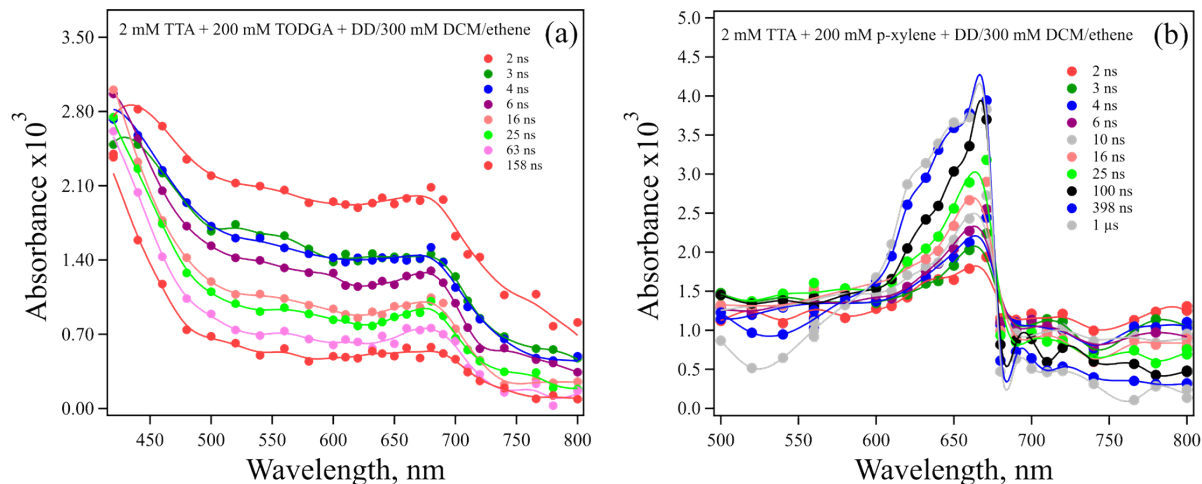


Fig. S7. Kinetic traces obtained for electron pulse-irradiated, aerated 2 mM MePTZ at 520 nm in absence and presence of 200 mM of TODGA/*p*-xylene in DD/0.3 M DCM (a) or DD/0.3 M DCM/ethene (b).

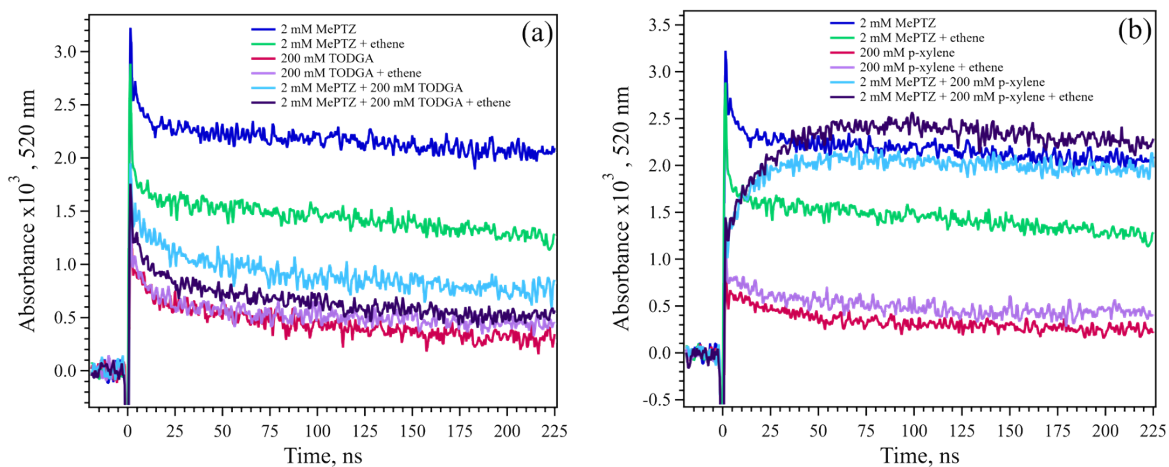


Fig. S8. Kinetic traces obtained for electron pulse irradiated, Ar saturated 0-10 mM TTA at 800 nm in DD/0.3 M DCM. Data were fit to a biexponential function to describe the geminate recombination with addition $k_{HT} = 2.1 \times 10^{10} \text{ M}^{-1}\text{s}^{-1}$ to describe the transfer to TTA.

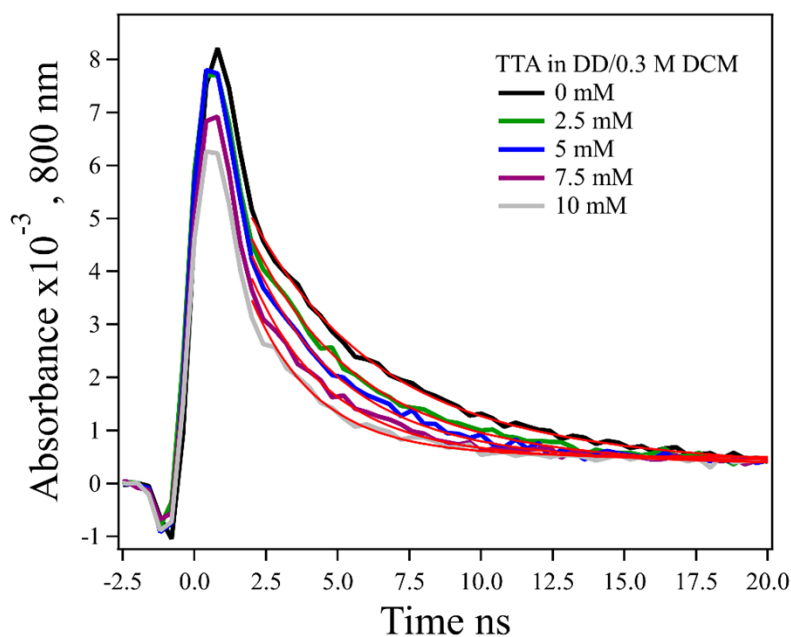


Fig. S9. Optimized structures after proton transfer from etheric carbon to oxygens: (a) bimolecular and (b) intramolecular. Such proton transfer reactions are energetically favorable because etheric protons of TODGA $^{\bullet+}$ are more acidic compared to neutral TODGA and oxygens make good receptors.

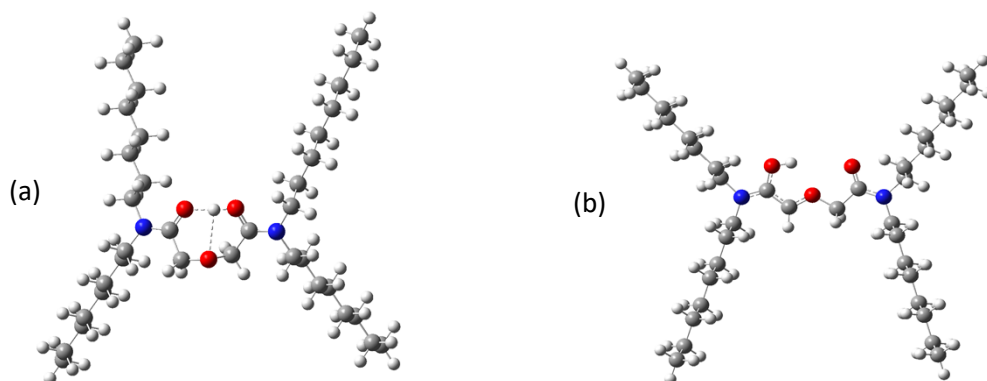


Fig. S10. Degradation of TODGA(-H) $\cdot$ to form *N,N*-dioctyl-2-oxoacetamide and *N,N*-dioctylacetamide radical.

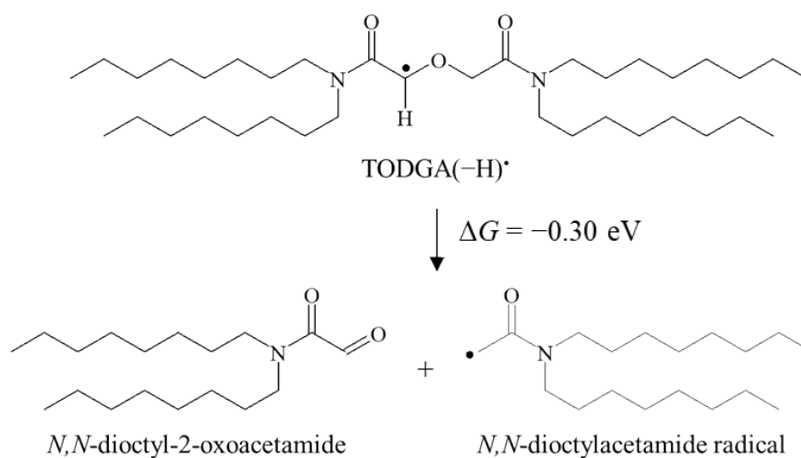
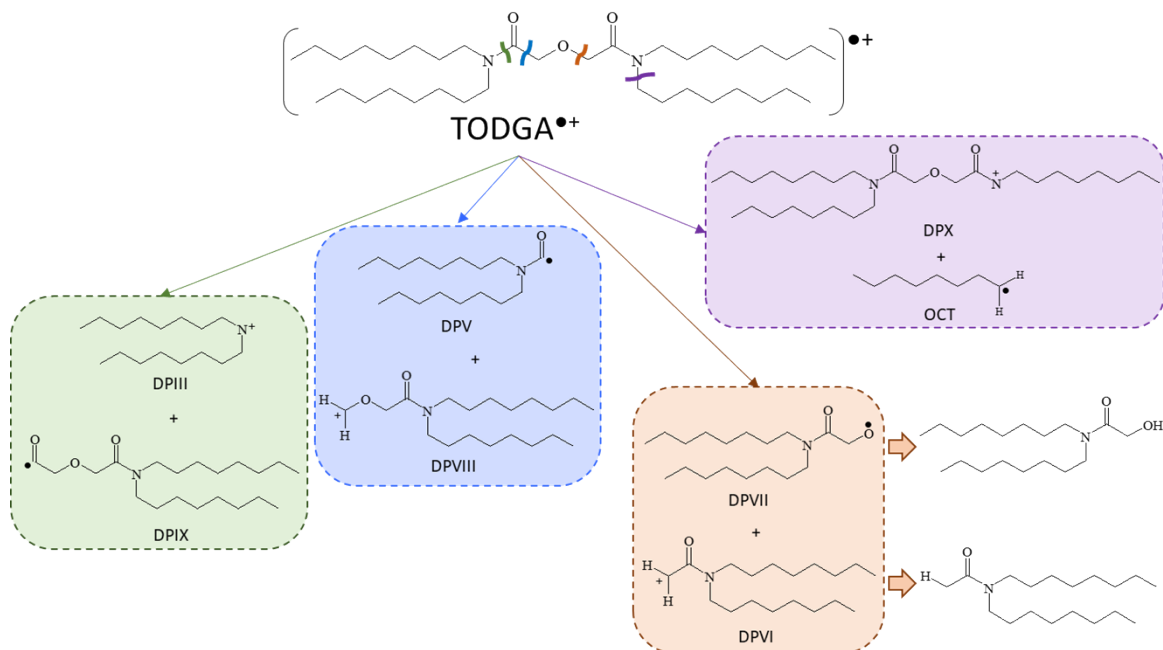


Fig. S11. Degradation scheme examined for the formation of products of TODGA $\bullet^+$. Free energy of reactions are provided in Table S6. Computed free energies of these reactions, suggests only one favorable degradation pathway ($\Delta G = -0.31 \text{ eV}$), where TODGA $\bullet^+$ breaks and gives the *N,N*-dioctylcarboxamide radical and 2-methoxy-*N,N*-dioctylacetamide cation (DPV $\cdot$ and DPVIII $^+$).



2) Tables S1-S6

Table S1. Calculated IPs of scavengers and indicators in DD using the B3LYP functional and 6-31+G* basis set.

Scavengers	Calculated IP (eV) in DD
DD	8.11
TODGA	6.92
<i>p</i> -Xylene	7.18
TTA	5.55
MePTZ	5.78

Table S2. Calculated free energy of reaction between DD^{•+} and TODGA in DD using the B3LYP functional and 6-31+G* basis set.

Reaction	ΔG , eV	TD-DFT, λ_{max} nm (Oscillator strength)
DD ^{•+} + TODGA $\rightarrow$ DD(-H) [•] + TODGA(+H) ⁺	-1.07	DD(-H) [•] = 248 (0.021) TODGA(+H) ⁺ = 197 (0.37)

Table S3. Fraction electron densities of TODGA, *p*-xylene, DD and DCM are calculated using densities of samples.

Sample	fraction of total e ⁻ density, TODGA	fraction of total e ⁻ density, DD	Fraction of total e ⁻ density, DCM
DD/0.5 M DCM	0	0.9514	0.0486
25 mM TODGA + DD/0.5 M DCM	0.0188	0.9328	0.0484
50 mM TODGA + DD/0.5 M DCM	0.0374	0.9144	0.0482
100 mM TODGA + DD/0.5 M DCM	0.0741	0.8781	0.0478
200 mM TODGA + DD/0.5 M DCM	0.1457	0.8073	0.0469
300 mM TODGA + DD/0.5 M DCM	0.2149	0.7389	0.0462
400 mM TODGA + DD/0.5 M DCM	0.2819	0.6728	0.0454
500 mM TODGA + DD/0.5 M DCM	0.3466	0.6088	0.0447

Sample	fraction of total e ⁻ density, <i>p</i> -xylene	fraction of total e ⁻ density, DD	Fraction of total e ⁻ density, DCM
DD/0.5 M DCM	0	0.9514	0.0486
25 mM <i>p</i> -xylene + DD/0.5 M DCM	0.0034	0.9481	0.0485
50 mM <i>p</i> -xylene + DD/0.5 M DCM	0.0067	0.9448	0.0485
100 mM <i>p</i> -xylene + DD/0.5 M DCM	0.0134	0.9383	0.0483
200 mM <i>p</i> -xylene + DD/0.5 M DCM	0.0266	0.9254	0.0481
300 mM <i>p</i> -xylene + DD/0.5 M DCM	0.0396	0.9126	0.0478
500 mM <i>p</i> -xylene + DD/0.5 M DCM	0.0653	0.8874	0.0473

Table S4(a). Homogenous hole transfer from TODGA^{•+}/*p*-xylene^{•+} to TTA

Samples	Abs at 100 ns, 670 nm	(TTA+TODGA/ <i>p</i> -xylene)-TODGA/ <i>p</i> -xylene at 100 ns	%TTA
2 mM TTA	0.00433		100
2 mM TTA+ethene	0.00320		100
200 mM TODGA	0.00015		
200 mM TODGA+ethene	0.00020		
2 mM TTA+200 mM TODGA	0.00057	0.00042	9.82
2 mM TTA+200 mM TODGA+ethene	0.00055	0.00035	10.91
200 mM <i>p</i> -xylene	0.00014		
200 mM <i>p</i> -xylene+ethene	0.00022		
2 mM TTA+200 mM <i>p</i> -xylene	0.00436	0.00422	97.40
2 mM TTA+200 mM <i>p</i> -xylene+ethene	0.00353	0.00332	103.66

Table S4(b). Homogenous hole transfer from TODGA^{•+}/*p*-xylene^{•+} to MePTZ

Samples	Abs at 50 ns, 520 nm	(MePTZ+TODGA/ <i>p</i> -xylene)-TODGA/ <i>p</i> -xylene at 50 ns	% MePTZ
2 mM MePTZ	0.00223		100
2 mM MePTZ+ethene	0.00154		100
200 mM TODGA	0.00053		
200 mM TODGA+ethene	0.00056		
2 mM MePTZ+200 mM TODGA	0.00099	0.00046	20.57
2 mM MePTZ+200 mM TODGA+ethene	0.00074	0.00018	11.54
200 mM <i>p</i> -xylene	0.00038		
200 mM <i>p</i> -xylene+ethene	0.00055		
2 mM MePTZ+200 mM <i>p</i> -xylene	0.00205	0.00167	74.98
2 mM MePTZ+200 mM <i>p</i> -xylene+ethene	0.00234	0.00179	116.89

Table S5. Fraction electron densities of solutes and solvents are calculated using densities of samples.

Sample	fraction of total e-density, TODGA	fraction of total e-density, DCM	Fraction of total e-density, TTA	Fraction of total e-density, DD
DD/0.3 M DCM	0	0.0295	0	0.9705
2 mM TTA + DD/0.3 M DCM	0	0.0294	0.00072	0.9699
200 mM TODGA + DD/0.3 M DCM	0.1453	0.0281	0	0.8266
2 mM TTA + 200 mM TODGA + DD/0.3 M DCM	0.1452	0.0281	0.00069	0.8261

Table S6. Possible degradation products of TODGA(–H)• (Fig. S10) and TODGA•+ (Fig. S11), the calculated free energies of reactions, and $\lambda_{\max}$ of transient species using b3lyp/6-31+g*.

TODGA(–H)• degradation reaction	ΔG , eV	TD-DFT, $\lambda_{\max}$, nm (Oscillator strength)
TODGA(–H)• $\rightarrow$ N,N-dioctyl-2-oxoacetamide + N,N-dioctylacetamide radical	–0.30	N,N-dioctyl-2-oxoacetamide = 296 (0.0581) N,N-dioctylacetamide radical = 572 (0.0146)
TODGA•+ degradation reactions	ΔG , eV	TD-DFT, $\lambda_{\max}$, nm (Oscillator strength)
TODGA•+ $\rightarrow$ DPX ⁺ + OCT•	0.96	
TODGA•+ $\rightarrow$ DPX• + OCT ⁺	1.92	
TODGA•+ $\rightarrow$ DPVII ⁺ + DPVI•	...	
TODGA•+ $\rightarrow$ DPVII• + DPVI ⁺	1.88	
TODGA•+ $\rightarrow$ DPV ⁺ + DPVIII•	0.89	
TODGA•+ $\rightarrow$ DPV• + DPVIII ⁺	–0.31	DPV• = 240 (0.030) DPVIII ⁺ = 229 (0.056)
TODGA•+ $\rightarrow$ DPIII ⁺ + DPIX•	2.86	
TODGA•+ $\rightarrow$ DPIII• + DPIX ⁺	...	
TODGA•+ $\rightarrow$ DPVII + DPVI•+	3.04	

3) Additional details Sections S1-S3

Section S1. Possible pathways of TTA^{•+} formation

There are three possible ways of TTA^{•+} formation; 1) direct ionization 2) oxidation by DD^{•+} and 3) Oxidation by TODGA^{•+}.

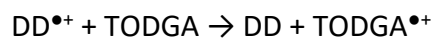
First, to calculate the contribution due to direct ionization, fraction electron densities were calculated with the help of densities of samples (Table S5). About 0.072% of the increase in TTA^{•+} signal with 200 mM TODGA can be explained by direct ionization.

Second, due to high IP of DD than TODGA and TTA, both can undergo oxidation by DD^{•+}. The amount of geminate DD^{•+} capture by TODGA was calculated from absorbance values of DD and DD+200 mM TODGA samples at 20 ps. The %geminate DD^{•+} capture by 200 mM TODGA is 50% (After direct ionization correction). The remaining 50% DD^{•+} can distribute between TODGA, TTA and DD^{•+} decay by diffusion. The details are provided in section S2.

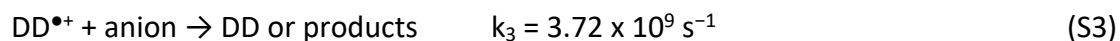
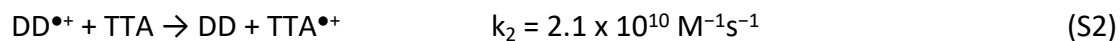
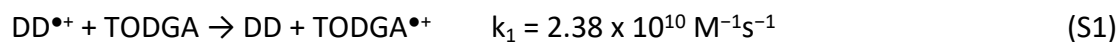
Third, the hole transfer from TODGA^{•+} to TTA was calculated by subtracting TTA^{•+} formation by direct ionization (0.072%) and transfer by DD^{•+} (0.25%) from total observed TTA^{•+} formation (From 2 mM TTA + 200 mM TODGA, total TTA^{•+} formation is ~10%). The percentage TTA^{•+} formation due to hole transfer from TODGA^{•+} is ~9.7%.

Section S2. Fraction of DD^{•+} holes distributed between TODGA, TTA and recombination products

Determination of the fraction of holes captured by Ultrafast hole capture:



TODGA quenches 50% of DD^{•+} after direct ionization correction.



The fractions for each reaction by diffusion are as follows:

Where, [TODGA] = 200 mM, [TTA] = 2 mM

$$f_1 = k_1 * [\text{TODGA}] / (k_1 * [\text{TODGA}] + k_2 * [\text{TTA}] + k_3) = 0.5586$$

$$f_2 = k_2 * [\text{TTA}] / (k_1 * [\text{TODGA}] + k_2 * [\text{TTA}] + k_3) = 0.0049$$

$$f_3 = k_3 / (k_1 * [\text{TODGA}] + k_2 * [\text{TTA}] + k_3) = 0.4365$$

However, 200 mM TODGA at 20 ps quenched 50% DD^{•+} signal. Then 50% fraction will distribute between TTA, TODGA and products according to fractions calculated above.

Fraction that goes to TODGA by geminate capture and diffusion = 0.50 + 0.50*0.5586 = 0.7793

Fraction that goes to TTA by diffusion = 0.50*0.0049 = 0.00245

Fraction that goes to Products by geminate recombination and diffusion = 0.50*0.4365 = 0.21825

Section S3. Fractions of TODGA^{•+} holes distribution to TTA and degradation products, and lifetime of TODGA^{•+}

TODGA^{•+} + TTA → TODGA + TTA^{•+} $k_1 = 2.1 \times 10^{10} \text{ M}^{-1}\text{s}^{-1}$ (Use as a proxy from DD+TTA rate constant) (S4)

TODGA^{•+} → Degradation products $k_2 = \text{Unknown}$
(S5)

The fractions for each reaction by diffusion are as follows;

Where, [TTA] = 2 mM

$f_1 = 0.1$ (Observed 10% hole transfer) – 7.2×10^{-4} (Fraction of direct ionization of TTA) – 0.00245
(Fraction of hole capture from DD^{•+} by TTA) = 0.09683

$$f_1 = k_1 * [\text{TTA}] / (k_1 * [\text{TTA}] + k_2)$$

$$k_2 = (k_1 * [\text{TTA}] / f_1) - k_1 * [\text{TTA}]$$

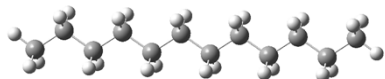
$$k_2 = 3.9 \times 10^8 \text{ s}^{-1}$$

$$\text{Lifetime of TODGA}^{\bullet+} = 1/k_2 = 2.6 \text{ ns}$$

4) Optimized geometries (XYZ) determined by computations

All structures are calculated using b3lyp/6-31+g* scrf(solvent=n-dodecane)

Dodecane

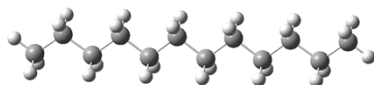


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H	0.55246900	7.16543000	-0.88563500
C	-0.84157000	5.73547600	0.00000000
H	-1.50086300	5.68723800	0.87917500
H	-1.50086300	5.68723800	-0.87917500
C	0.08957500	4.51519800	0.00000000
H	0.74970900	4.56474200	-0.87972900
H	0.74970900	4.56474200	0.87972900
C	-0.65400100	3.17241500	0.00000000
H	-1.31405200	3.12403200	-0.87971100
H	-1.31405200	3.12403200	0.87971100
C	0.27794700	1.95263300	0.00000000
H	0.93799600	2.00112600	0.87968000
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C	-0.46595200	0.60989100	0.00000000
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H	-1.12602200	0.56149400	0.87968400
C	0.46595200	-0.60989100	0.00000000
H	1.12602200	-0.56149400	0.87968400
H	1.12602200	-0.56149400	-0.87968400
C	-0.27794700	-1.95263300	0.00000000
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H	-0.93799600	-2.00112600	0.87968000
C	0.65400100	-3.17241500	0.00000000
H	1.31405200	-3.12403200	0.87971100
H	1.31405200	-3.12403200	-0.87971100
C	-0.08957500	-4.51519800	0.00000000
H	-0.74970900	-4.56474200	-0.87972900
H	-0.74970900	-4.56474200	0.87972900
C	0.84157000	-5.73547600	0.00000000
H	1.50086300	-5.68723800	0.87917500
H	1.50086300	-5.68723800	-0.87917500
C	0.08957500	-7.07202800	0.00000000

H	-0.55246900	-7.16543000	-0.88563500
H	-0.55246900	-7.16543000	0.88563500
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Dodecane radical cation

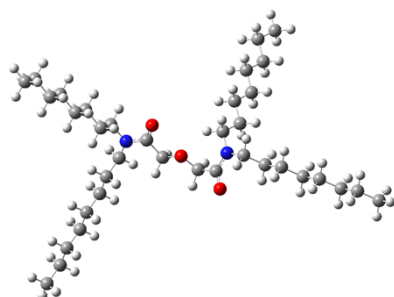


1 2

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H	0.52788100	7.02173100	-0.88901800
C	-0.88114600	5.59563400	0.00000000
H	-1.52857800	5.53832000	0.88314400
H	-1.52857800	5.53832000	-0.88314400
C	0.10508100	4.39863600	0.00000000
H	0.74929500	4.44533100	-0.88552800
H	0.74929500	4.44533100	0.88552800
C	-0.70332100	3.07259300	0.00000000
H	-1.34257500	3.01921500	-0.88714600
H	-1.34257500	3.01921500	0.88714600
C	0.32019000	1.89812900	0.00000000
H	0.95645100	1.94468500	0.88858100
H	0.95645100	1.94468500	-0.88858100
C	-0.51969800	0.58257400	0.00000000
H	-1.15398200	0.53298100	-0.88929900
H	-1.15398200	0.53298100	0.88929900
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H	1.15398200	-0.53298100	0.88929900
H	1.15398200	-0.53298100	-0.88929900
C	-0.32019000	-1.89812900	0.00000000
H	-0.95645100	-1.94468500	-0.88858100
H	-0.95645100	-1.94468500	0.88858100
C	0.70332100	-3.07259300	0.00000000
H	1.34257500	-3.01921500	0.88714600
H	1.34257500	-3.01921500	-0.88714600
C	-0.10508100	-4.39863600	0.00000000
H	-0.74929500	-4.44533100	-0.88552800
H	-0.74929500	-4.44533100	0.88552800
C	0.88114600	-5.59563400	0.00000000
H	1.52857800	-5.53832000	0.88314400
H	1.52857800	-5.53832000	-0.88314400

C	0.10508100	-6.92399900	0.00000000
H	-0.52788100	-7.02173100	-0.88901800
H	-0.52788100	-7.02173100	0.88901800
H	0.82195400	-7.75643100	0.00000000

TODGA

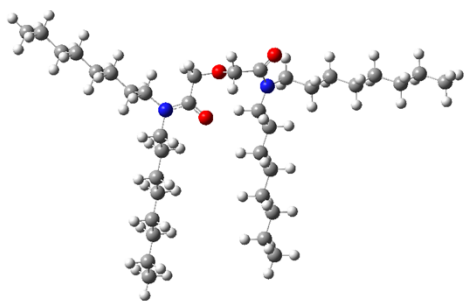


O 1			
O	0.11308700	0.52641600	0.19827100
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H	-1.56429600	1.49265300	0.91042800
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H	1.50629400	1.11627700	1.62510600
H	0.66338000	2.44708800	0.78685900
C	-1.94807800	-0.63877800	0.58221800
C	2.20779200	1.60607000	-0.38871100
N	-3.22694600	-0.63862100	1.06510300
N	2.99283000	0.53699700	-0.68969700
O	2.37509500	2.71682400	-0.90978300
O	-1.51923600	-1.53730800	-0.14122600
C	-3.76438100	0.37706500	1.97918400
H	-4.34942000	-0.14816200	2.74517900
C	-4.09721500	-1.76173100	0.67776700
H	-4.90008300	-1.81795100	1.42155000
C	2.83310500	-0.80367300	-0.10700400
H	2.84427500	-1.52508400	-0.93468100
C	4.02863800	0.72677100	-1.71864700
H	4.27896200	-0.26642100	-2.10805900
C	-4.69074900	-1.64876200	-0.73441300
H	-5.29373500	-0.73382100	-0.80983400
H	-3.86801700	-1.55193500	-1.45226900
C	-5.55301900	-2.86583900	-1.09609600
H	-4.94376100	-3.77834800	-1.01475200
H	-6.36707300	-2.97259200	-0.36207300

C	-6.15294300	-2.78408400	-2.50690200
H	-6.76043900	-1.86998100	-2.59055500
H	-5.33850300	-2.67835400	-3.23895000
C	-7.01401100	-3.99908700	-2.87884100
H	-7.82819800	-4.10543300	-2.14544500
H	-6.40605100	-4.91281700	-2.79540400
C	-7.61262200	-3.91782800	-4.28988500
H	-6.79890500	-3.81167200	-5.02357200
H	-8.22086800	-3.00405300	-4.37457400
C	-8.47338500	-5.13218700	-4.66478600
H	-9.28762100	-5.23837300	-3.93284700
H	-7.86608500	-6.04538300	-4.58101500
C	-9.06582300	-5.04227900	-6.07639700
H	-8.27469700	-4.97032900	-6.83404400
H	-9.67423700	-5.92383600	-6.31266100
H	-9.70643100	-4.15696900	-6.18165800
H	-3.50863200	-2.68252200	0.74931400
H	-2.93874300	0.85565700	2.51301200
C	-4.63860400	1.44678000	1.30630400
H	-4.05990800	1.93780200	0.51159300
H	-5.49172300	0.96172400	0.81433900
C	-5.15077100	2.49460300	2.30420000
H	-5.71075000	1.99125000	3.10706000
H	-4.29438900	2.98661000	2.79010200
C	-6.04534300	3.56099000	1.65643800
H	-5.48604900	4.06342900	0.85305500
H	-6.90151700	3.06840400	1.17132000
C	-6.56183900	4.61227500	2.64841800
H	-7.11921300	4.10881400	3.45314900
H	-5.70535100	5.10620600	3.13217900
C	-7.45908400	5.67618400	2.00117700
H	-8.31620700	5.18294300	1.51748700
H	-6.90244100	6.17960700	1.19595200
C	-7.97663900	6.72941300	2.99060000
H	-8.53313100	6.22706000	3.79548200
H	-7.12074300	7.22380800	3.47305100
C	-8.87262400	7.78724600	2.33506700
H	-9.75609100	7.32738000	1.87340400
H	-9.22474800	8.52348100	3.06780800
H	-8.33329100	8.33110700	1.54871000
H	3.58611500	1.30559100	-2.53636000
C	5.29864000	1.43722100	-1.22591300
H	5.75365000	0.85812600	-0.41112800
H	5.01668800	2.41189200	-0.81103200

C	6.32127100	1.63112700	-2.35396200
H	6.58404400	0.65251500	-2.78519700
H	5.85827600	2.21062600	-3.16652700
C	7.60326000	2.34062000	-1.89568200
H	8.06695800	1.76266900	-1.08158300
H	7.34018500	3.31865500	-1.46561200
C	8.62815700	2.54114500	-3.02058700
H	8.16411900	3.11963000	-3.83389300
H	8.88942600	1.56262200	-3.45209800
C	9.91060900	3.25046400	-2.56431100
H	10.37612300	2.67233400	-1.75111800
H	9.65018100	4.22906400	-2.13258000
C	10.93559700	3.45290100	-3.68882200
H	10.47151200	4.03153400	-4.50093900
H	11.19661800	2.47547000	-4.12058900
C	12.21338800	4.16205600	-3.22397800
H	12.71956900	3.59004900	-2.43538400
H	12.92343100	4.29101500	-4.05002600
H	11.98894600	5.15735600	-2.81879700
H	1.84002900	-0.87539600	0.33661600
C	3.91401500	-1.17661500	0.91873600
H	4.90531700	-1.14080500	0.44719300
H	3.92395700	-0.42546600	1.72162600
C	3.68525300	-2.57315200	1.51430500
H	2.69541500	-2.60803700	1.99348200
H	3.65562300	-3.31468800	0.70182500
C	4.75780200	-2.98266100	2.53338900
H	5.74691600	-2.94870900	2.05182600
H	4.78831700	-2.24116200	3.34628700
C	4.53393900	-4.37906200	3.13026900
H	3.54551000	-4.41259700	3.61344600
H	4.50097100	-5.11962200	2.31669500
C	5.60777400	-4.79180400	4.14632200
H	5.64223100	-4.05100100	4.96004200
H	6.59641200	-4.76015700	3.66301200
C	5.38456100	-6.18743100	4.74518600
H	5.35059400	-6.92820100	3.93289800
H	4.39743700	-6.21953600	5.22929800
C	6.46233400	-6.59145000	5.75848500
H	6.27351100	-7.59179700	6.16676500
H	7.45747800	-6.60288100	5.29511500
H	6.49751100	-5.88857900	6.60107400

TODGA radical cation



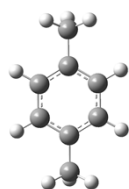
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O	0.07113400	-2.65435400	-1.27071100
C	-1.28133600	-2.38635100	-1.60513000
H	-1.51219800	-2.76720900	-2.61045400
H	-1.87793800	-2.95195700	-0.88490100
C	1.00356200	-2.42336000	-2.31416200
H	0.92213500	-1.40449600	-2.71503200
H	0.88481700	-3.14303100	-3.13313300
C	-1.59386500	-0.87865200	-1.50606800
C	2.38467500	-2.65600000	-1.72690100
N	-2.87912500	-0.48069100	-1.62063100
N	2.70284100	-1.97256500	-0.49205800
O	3.21286500	-3.40064800	-2.19922000
O	-0.65891200	-0.07690900	-1.33438600
C	-4.00125000	-1.40406000	-1.86588700
H	-4.62209600	-0.95823200	-2.65190700
C	-3.17100200	0.96568600	-1.53160700
H	-4.14299400	1.12127100	-2.01006300
C	2.19346400	-0.64863500	-0.22807600
H	2.38412000	-0.41808200	0.82173900
C	3.66904200	-2.59862100	0.39850900
H	3.32485700	-2.41120600	1.42103400
C	-3.18636100	1.51988700	-0.09912700
H	-3.93897600	0.98569900	0.49464000
H	-2.21243400	1.32727300	0.36626200
C	-3.48412400	3.02600400	-0.07321800
H	-2.72823700	3.55711400	-0.67064000
H	-4.45205600	3.21729800	-0.56047600
C	-3.51023300	3.60981200	1.34669200
H	-4.26322900	3.07427100	1.94422800
H	-2.54143000	3.42140300	1.83360700
C	-3.81222300	5.11438000	1.38416800
H	-4.77950300	5.30194000	0.89397600
H	-3.05804600	5.65101000	0.78864300

C	-3.84423000	5.69687000	2.80397400
H	-2.87646200	5.51136100	3.29500000
H	-4.59740100	5.15904800	3.39993700
C	-4.14966400	7.20064700	2.84497200
H	-5.11708700	7.38644000	2.35611600
H	-3.39765400	7.73899200	2.24968100
C	-4.17958400	7.77344000	4.26705300
H	-3.21439600	7.63437200	4.77121500
H	-4.40008100	8.84759400	4.26073400
H	-4.94674500	7.27944800	4.87724500
H	-2.41828400	1.49547000	-2.12345400
H	-3.61411900	-2.33792500	-2.28027000
C	-4.85899100	-1.70334000	-0.62703600
H	-4.21488500	-2.08971300	0.17518300
H	-5.30109300	-0.77180300	-0.25207200
C	-5.97486700	-2.71245900	-0.93460400
H	-6.60134900	-2.32604500	-1.75226600
H	-5.52897500	-3.64796300	-1.30446100
C	-6.86163700	-3.02033100	0.28040600
H	-6.23371600	-3.39750600	1.10159400
H	-7.31410600	-2.08574100	0.64386900
C	-7.97109900	-4.03860500	-0.01763800
H	-8.59644700	-3.66289500	-0.84157300
H	-7.51733100	-4.97392700	-0.37903400
C	-8.86164200	-4.34425100	1.19458600
H	-9.31719200	-3.40945000	1.55525000
H	-8.23646000	-4.71821200	2.01987000
C	-9.97040200	-5.36436400	0.90070600
H	-10.59634700	-4.99110700	0.07707000
H	-9.51593200	-6.29896600	0.54065100
C	-10.85420200	-5.66326000	2.11755500
H	-11.34872300	-4.75333700	2.48132200
H	-11.63602700	-6.39252500	1.87405700
H	-10.26249200	-6.07318100	2.94628100
H	3.66827500	-3.66997100	0.19607300
C	5.11490500	-2.03802900	0.22603100
H	5.12363300	-0.96739100	0.45885700
H	5.41004800	-2.16174300	-0.82135200
C	6.08438900	-2.78408400	1.15391200
H	5.75769400	-2.67121200	2.19713100
H	6.05958700	-3.85856700	0.92738900
C	7.52409700	-2.26363500	1.00759500
H	7.54634400	-1.18525900	1.22154200
H	7.84880000	-2.38219200	-0.03593900

C	8.51301300	-2.98721000	1.93487200
H	8.48403200	-4.06655900	1.72539600
H	8.18758600	-2.86535600	2.97860800
C	9.95457700	-2.47940700	1.78892400
H	9.98192800	-1.39799900	1.99121200
H	10.28036300	-2.60547500	0.74545700
C	10.94779700	-3.19231400	2.71773700
H	10.91871800	-4.27307500	2.51731000
H	10.62360700	-3.06438300	3.76069900
C	12.38577000	-2.68267900	2.56382800
H	12.45293800	-1.61073900	2.78992300
H	13.06923600	-3.20948400	3.24024300
H	12.75105900	-2.82995200	1.53939800
H	1.10942000	-0.63598900	-0.43512000
C	2.85275300	0.44019900	-1.14611600
H	3.94126800	0.38474000	-1.03913900
H	2.61365500	0.22736700	-2.19453600
C	2.34017500	1.83328200	-0.75766100
H	1.24796000	1.85748800	-0.85248400
H	2.57567200	2.02826400	0.29809600
C	2.96802400	2.93145200	-1.63250900
H	4.06384700	2.88348000	-1.55339100
H	2.72331300	2.74095000	-2.68735900
C	2.49247900	4.34093200	-1.24598200
H	1.39639300	4.38776800	-1.32460600
H	2.73484000	4.52917400	-0.18956500
C	3.11322600	5.44429300	-2.11485700
H	2.87252300	5.25371100	-3.17163100
H	4.20981300	5.39563200	-2.03633700
C	2.64175200	6.85575300	-1.73629700
H	2.88253300	7.04694900	-0.68050300
H	1.54596900	6.90443700	-1.81479400
C	3.26462100	7.95223700	-2.60875700
H	2.90680500	8.94597700	-2.31447900
H	4.35890800	7.95322000	-2.52419700
H	3.01337400	7.80739600	-3.66733100

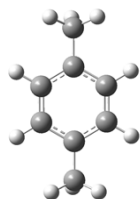
p-Xylene



0 1

C	-0.69861900	1.19923300	-0.01234100
C	-1.42538600	-0.00020100	-0.00809000
C	-0.69880000	-1.19945900	-0.01232500
C	0.69880000	-1.19945900	-0.01232500
C	1.42538600	-0.00020100	-0.00809000
C	0.69861900	1.19923300	-0.01234100
H	-1.23176200	2.14827800	-0.02161900
H	-1.23187800	-2.14852400	-0.02163800
H	1.23187800	-2.14852400	-0.02163800
H	1.23176200	2.14827800	-0.02161900
C	-2.93748500	0.00023800	0.02218100
H	-3.31443300	0.01239600	1.05421600
H	-3.34874100	0.88082100	-0.48406700
H	-3.34870700	-0.89183800	-0.46344400
C	2.93748500	0.00023800	0.02218100
H	3.34874100	0.88082100	-0.48406700
H	3.31443300	0.01239600	1.05421600
H	3.34870700	-0.89183800	-0.46344400

p-Xylene radical cation

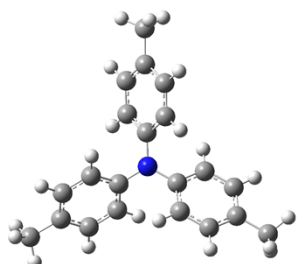


1 2

C	-0.68532200	1.23545300	-0.02666100
C	-1.41554900	-0.00000700	-0.01890200
C	-0.68532400	-1.23546100	-0.02666400
C	0.68532400	-1.23546100	-0.02666400
C	1.41555000	-0.00000700	-0.01891200
C	0.68532200	1.23545200	-0.02666800
H	-1.23696700	2.17111400	-0.02913500
H	-1.23696200	-2.17112700	-0.02914700
H	1.23696200	-2.17112700	-0.02913100
H	1.23696700	2.17111400	-0.02914400
C	-2.89753200	0.00000600	0.03742100
H	-3.21061700	0.00019600	1.09745100
H	-3.32751300	0.89804100	-0.41530200
H	-3.32752900	-0.89816600	-0.41500500
C	2.89753200	0.00000600	0.03742400

H	3.32751600	0.89804000	-0.41529800
H	3.21060900	0.00019900	1.09745700
H	3.32753300	-0.89816700	-0.41499700

TTA

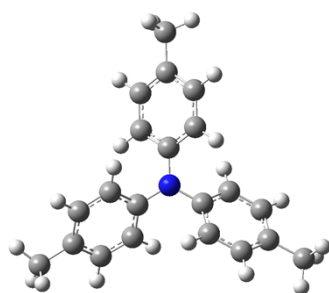


O 1

N	-0.00028400	-0.00001500	0.00904100
C	0.53899600	1.31591000	0.00451700
C	1.64128400	1.64442400	0.81051900
C	-0.01412300	2.31785800	-0.80945300
C	2.17322900	2.93405200	0.79193600
H	2.08480100	0.88429700	1.44706100
C	0.51702500	3.60798300	-0.80482800
H	-0.86099900	2.08270000	-1.44759400
C	1.62122500	3.94579100	-0.00812400
H	3.03074100	3.15849000	1.42363900
H	0.06976400	4.36347100	-1.44821100
C	0.86982400	-1.12509200	0.00398000
C	0.60450700	-2.24305400	0.81149700
C	2.01284300	-1.14773600	-0.81187100
C	1.45579700	-3.34835500	0.79321500
H	-0.27474500	-2.24664200	1.44912800
C	2.86499800	-2.25237700	-0.80682000
H	2.23126900	-0.29762900	-1.45166400
C	2.60706800	-3.37651100	-0.00798000
H	1.22278200	-4.20247600	1.42637000
H	3.74188600	-2.24346100	-1.45163200
C	-1.40949700	-0.19102300	0.00433900
C	-2.24509700	0.59885900	0.81063000
C	-2.00071800	-1.17059300	-0.81038900
C	-3.62794300	0.41442400	0.79230100
H	-1.80872400	1.36289400	1.44741800
C	-3.38344200	-1.35583600	-0.80557600
H	-1.37364900	-1.78558600	-1.44934400
C	-4.22809100	-0.56920800	-0.00792600

H	-4.25097700	1.04429300	1.42459000
H	-3.81423700	-2.12041600	-1.44950300
C	2.17688200	5.35180500	0.00883700
H	2.00545600	5.86141200	-0.94608000
H	1.70261800	5.95975400	0.79189000
H	3.25515200	5.35478800	0.20441500
C	-5.72342400	-0.79183200	0.00902600
H	-6.00966500	-1.52620600	0.77483100
H	-6.26449700	0.13513700	0.22985600
H	-6.08264300	-1.17128000	-0.95434200
C	3.54821500	-4.55964200	0.00947900
H	4.04941700	-4.68695800	-0.95681900
H	4.33291300	-4.43512000	0.76871100
H	3.01797500	-5.49043100	0.24013900

TTA radical cation

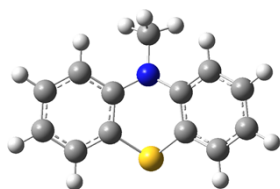


1 2

N	0.00057600	-0.00116100	-0.00061500
C	-0.15183600	1.40352900	-0.00205100
C	0.71398800	2.21141000	0.76397900
C	-1.16867100	2.00655200	-0.77127400
C	0.55388100	3.59022200	0.75842100
H	1.48145400	1.75211100	1.37816800
C	-1.30495200	3.38795500	-0.77026700
H	-1.81660400	1.39334000	-1.38898600
C	-0.45433800	4.20946800	-0.00526400
H	1.21571300	4.20172000	1.36569000
H	-2.07623300	3.84304300	-1.38578300
C	1.29324700	-0.57227900	-0.00255900
C	1.56195900	-1.72312400	0.76712400
C	2.32211800	0.00457500	-0.77567100
C	2.83687700	-2.27232300	0.76228700
H	0.78122800	-2.15733000	1.38267300
C	3.58678700	-0.56748300	-0.77537200

H	2.11377800	0.87155700	-1.39383500
C	3.87540800	-1.71105800	-0.00569300
H	3.03703700	-3.14850000	1.37308300
H	4.36521200	-0.12874200	-1.39370200
C	-1.14029300	-0.83575800	0.00089900
C	-2.27100000	-0.49034800	0.76952300
C	-1.15673700	-2.01519600	-0.77195500
C	-3.38642400	-1.31658600	0.76260000
H	-2.25571500	0.40357700	1.38416400
C	-2.28682700	-2.82158300	-0.77346800
H	-0.30232000	-2.26901900	-1.39069000
C	-3.42178500	-2.49641300	-0.00557100
H	-4.24576800	-1.04925400	1.37149500
H	-2.29794000	-3.71485800	-1.39225000
C	-0.63380900	5.70410300	0.01543500
H	-1.04014200	6.07261500	-0.93169100
H	-1.33790300	5.99415300	0.80757700
H	0.31082300	6.21961400	0.21426900
C	-4.62802100	-3.39715300	0.01350300
H	-4.53106500	-4.14942000	0.80849600
H	-5.54679600	-2.83502900	0.20731600
H	-4.74156400	-3.93617600	-0.93223000
C	5.26054200	-2.30044500	0.01635300
H	5.78770000	-2.12248500	-0.92609100
H	5.85858700	-1.84288500	0.81655300
H	5.23578900	-3.37829100	0.20419100

MePTZ

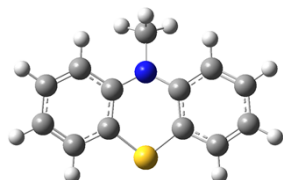


0 1

C	3.52339800	0.71896700	0.65414700
C	2.32074900	1.33677200	0.29719400
C	1.21795000	0.57341200	-0.12163900
C	1.34870500	-0.83076800	-0.14516500
C	2.53935500	-1.44364100	0.24897200
C	3.63942200	-0.67116800	0.63423900
C	-1.34869700	-0.83077000	-0.14513800
C	-1.21796100	0.57341500	-0.12166700

C	-2.32077200	1.33676700	0.29714000
H	-2.24705400	2.41737500	0.34903800
C	-3.52340000	0.71894800	0.65414900
C	-3.63941800	-0.67118600	0.63424700
C	-2.53933600	-1.44365600	0.24900500
H	4.36438900	1.33484100	0.96173100
H	2.24700700	2.41737700	0.34912700
H	2.60704600	-2.52829800	0.23631000
H	4.56944700	-1.15428400	0.92004800
H	-4.36439600	1.33482000	0.96172500
H	-4.56943600	-1.15430800	0.92006800
H	-2.60701700	-2.52831300	0.23635100
S	0.00001100	-1.81363400	-0.77272500
N	-0.00000300	1.17105500	-0.52361100
C	-0.00001100	2.59637400	-0.82474700
H	-0.00005000	3.23496200	0.07272200
H	0.88416800	2.83290700	-1.42130500
H	-0.88416400	2.83287700	-1.42135900

MePTZ radical cation

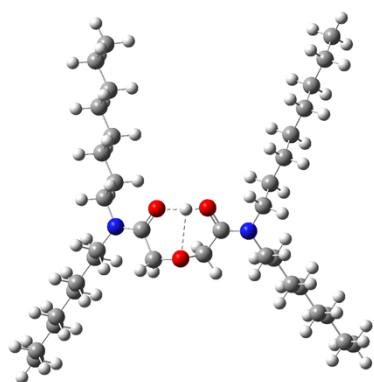


1 2

C	3.63673800	0.72865500	0.32506900
C	2.40522600	1.34590900	0.19152300
C	1.22998000	0.58493700	-0.01971200
C	1.35547600	-0.83221800	-0.06065100
C	2.61766000	-1.44172600	0.06383600
C	3.75259100	-0.67169700	0.25053800
C	-1.35547000	-0.83222400	-0.06063600
C	-1.22997600	0.58493100	-0.01969600
C	-2.40522300	1.34590400	0.19152000
H	-2.34875200	2.42216100	0.28404600
C	-3.63673800	0.72865100	0.32505900
C	-3.75258700	-0.67170100	0.25053800
C	-2.61765400	-1.44173000	0.06385100
H	4.51780700	1.33804100	0.49940100
H	2.34875200	2.42216600	0.28406000
H	2.68953000	-2.52456100	0.02242700

H	4.72213600	-1.14833800	0.35208100
H	-4.51780900	1.33803800	0.49937400
H	-4.72213400	-1.14834100	0.35207200
H	-2.68952500	-2.52456500	0.02244300
S	0.00000000	-1.89567400	-0.32137300
N	0.00000200	1.22117700	-0.18939800
C	-0.00001500	2.66360200	-0.50774300
H	-0.00010000	3.27191800	0.40369000
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H	-0.87931300	2.89410000	-1.10647800

TODGA(+H)⁺



1 1

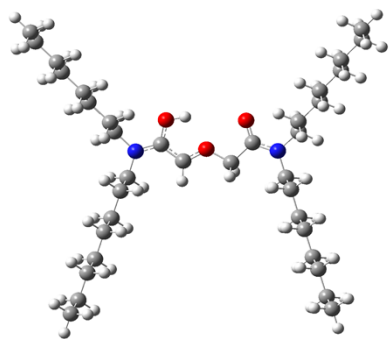
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H	0.11089700	1.34025900	1.18732100
C	1.84759300	0.85181900	2.93453800
H	2.42053100	0.99005400	3.85556700
H	2.32071200	1.45679200	2.14951200
C	-1.62232900	0.96650300	2.35781600
C	1.83205400	-0.63769900	2.54349000
N	-2.79447900	1.55395800	2.25749600
N	2.98917800	-1.26255000	2.29742300
O	0.73669900	-1.24832500	2.47041100
O	-1.57795800	-0.29599100	2.63561600
C	-2.95101500	3.00772500	1.98391700
H	-3.92519200	3.28478800	2.39208700
C	-4.02770800	0.73000300	2.41918800
H	-4.80847600	1.41066300	2.76563400
C	4.30523600	-0.59803500	2.37331600
H	4.97902000	-1.28352300	2.89928000

C	2.95640900	-2.70773500	1.96961500
H	3.95896000	-3.09292700	2.17672300
C	-4.45915600	0.01146000	1.13352100
H	-4.67512900	0.74819800	0.34936600
H	-3.63228800	-0.61269700	0.77298300
C	-5.69747200	-0.86559500	1.37287300
H	-5.47428400	-1.59974100	2.16051700
H	-6.52138400	-0.24347900	1.75246500
C	-6.15797700	-1.60181900	0.10669200
H	-6.38622600	-0.86537900	-0.67837300
H	-5.32854000	-2.21435000	-0.27715200
C	-7.38419700	-2.49637200	0.33502900
H	-8.21366300	-1.88449600	0.72058200
H	-7.15454300	-3.23186300	1.12070900
C	-7.84432200	-3.23398800	-0.92996100
H	-7.01295400	-3.84200400	-1.31843300
H	-8.07806500	-2.49830600	-1.71473400
C	-9.06553400	-4.13624000	-0.70453700
H	-9.89682500	-3.52970100	-0.31649400
H	-8.83155500	-4.87182600	0.07886900
C	-9.51792900	-4.86903300	-1.97317900
H	-8.71930100	-5.51131000	-2.36637200
H	-10.39014900	-5.50421300	-1.77803000
H	-9.79279000	-4.15944600	-2.76427000
H	-3.83475900	0.00438400	3.21185100
H	-2.20569000	3.55334900	2.56816600
C	-2.87158800	3.38486600	0.49947600
H	-1.90609500	3.06303200	0.08451500
H	-3.64695900	2.84356300	-0.05647000
C	-3.04370900	4.89739800	0.29371600
H	-4.00448100	5.21626000	0.72318800
H	-2.26250900	5.43432800	0.85235200
C	-2.98659200	5.31178600	-1.18370500
H	-2.02894200	4.98525600	-1.61633700
H	-3.77284900	4.77962600	-1.73938900
C	-3.14961800	6.82339800	-1.39510100
H	-4.10460900	7.14979200	-0.95671300
H	-2.36050900	7.35451600	-0.84139200
C	-3.10136300	7.24178300	-2.87108500
H	-3.89252400	6.71314300	-3.42431800
H	-2.14767700	6.91266800	-3.31149500
C	-3.26018900	8.75346900	-3.08508200
H	-4.21300000	9.08275700	-2.64572000
H	-2.46943200	9.28214000	-2.53286800

C	-3.21127200	9.16282500	-4.56192700
H	-4.01243700	8.67816300	-5.13463000
H	-3.32683400	10.24678500	-4.67956800
H	-2.25583500	8.87776300	-5.02107200
H	2.26182300	-3.18860400	2.66478600
C	2.55254500	-3.03428700	0.52560000
H	3.24376600	-2.54637500	-0.17366700
H	1.55331600	-2.62822800	0.32973600
C	2.55270500	-4.55036800	0.28106200
H	3.55581000	-4.95303300	0.48707900
H	1.87430300	-5.03349700	0.99963900
C	2.13576800	-4.93689800	-1.14463700
H	2.80695600	-4.44673000	-1.86590600
H	1.12783400	-4.54413600	-1.34639500
C	2.14894600	-6.45223500	-1.38871300
H	1.48066100	-6.94157500	-0.66404900
H	3.15781600	-6.84218500	-1.18561200
C	1.73048600	-6.84972100	-2.81069300
H	2.39701700	-6.35908900	-3.53651700
H	0.71984900	-6.46338900	-3.01393700
C	1.74926100	-8.36525400	-3.05362100
H	1.08393700	-8.85602000	-2.32829100
H	2.75916500	-8.75086100	-2.85147300
C	1.32963500	-8.75554700	-4.47574500
H	1.99659600	-8.30655000	-5.22306300
H	1.35634100	-9.84271300	-4.61626700
H	0.30912200	-8.41593800	-4.69530000
H	4.22266000	0.28906700	3.00489200
C	4.89802800	-0.21566400	1.00941800
H	5.04131700	-1.11961700	0.40441400
H	4.18130900	0.41553800	0.46503200
C	6.23577900	0.52444800	1.15501500
H	6.09355800	1.41427800	1.78677700
H	6.95259100	-0.11834700	1.68677300
C	6.83764200	0.95317500	-0.19091000
H	6.98347500	0.06499700	-0.82336200
H	6.11688500	1.59340100	-0.72191600
C	8.17072500	1.70125800	-0.05065900
H	8.02616600	2.58206800	0.59335500
H	8.89515800	1.05699900	0.46988500
C	8.76422300	2.14976400	-1.39329400
H	8.03873200	2.79362600	-1.91400000
H	8.91050100	1.27006200	-2.03838100
C	10.09580600	2.90095000	-1.25542500

H	10.82247900	2.25692800	-0.73919200
H	9.95076500	3.77846300	-0.60839500
C	10.67832200	3.35066400	-2.60063600
H	11.62707500	3.88379500	-2.46671200
H	10.86842200	2.49209000	-3.25751100
H	9.98892400	4.02423300	-3.12612900
H	-0.59151400	-0.65770600	2.65457100

TODGA(-H)(+H)*+



1 2

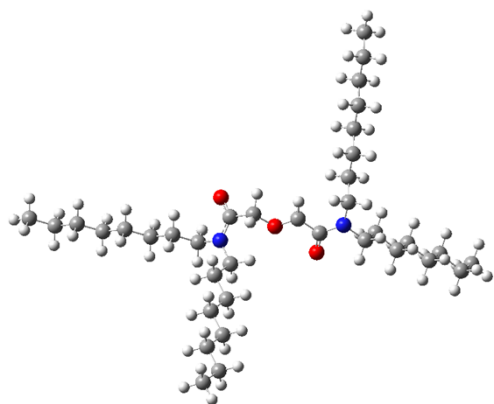
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C	1.16532600	0.40561000	2.50047700
H	1.22827200	0.97846900	3.43210800
H	1.16385700	1.08686700	1.64414500
C	-2.33137900	-0.63000900	2.34368100
C	2.28043000	-0.66017600	2.40262500
N	-3.61395700	-0.29031600	2.25347700
N	3.55059200	-0.21306500	2.27161500
O	1.97176600	-1.85168300	2.45170200
O	-2.06260000	-1.93472100	2.39079700
C	-4.05484300	1.12231600	2.26806500
H	-4.97725700	1.14627800	2.85592300
C	-4.64318300	-1.35559800	2.12509400
H	-5.59329100	-0.89359300	2.40284900
C	3.93057600	1.20819000	2.24319800
H	4.78181600	1.33198100	2.92380000
C	4.62204000	-1.22804500	2.18269200
H	5.55577400	-0.72645500	2.45747600
C	-4.73193300	-1.97462200	0.72030000
H	-4.96957100	-1.19376200	-0.01238600
H	-3.75773300	-2.39303800	0.44332500

C	-5.79851700	-3.07870100	0.66623400
H	-5.55762800	-3.85471000	1.40708600
H	-6.77433700	-2.66316500	0.95753600
C	-5.91404200	-3.72108000	-0.72362000
H	-6.15564600	-2.94362900	-1.46375800
H	-4.93548500	-4.13056500	-1.01498900
C	-6.97005300	-4.83282700	-0.79298200
H	-7.94796300	-4.42399200	-0.49708400
H	-6.72640200	-5.61084700	-0.05397300
C	-7.08872100	-5.47347200	-2.18268300
H	-6.10982900	-5.87962100	-2.47997000
H	-7.33447100	-4.69555700	-2.92169800
C	-8.14047200	-6.58900400	-2.25631000
H	-9.11910000	-6.18374700	-1.96037800
H	-7.89519300	-7.36645900	-1.51818100
C	-8.25082800	-7.22349200	-3.64780500
H	-7.29616500	-7.66806300	-3.95738500
H	-9.00877700	-8.01558800	-3.66670600
H	-8.52966400	-6.47710600	-4.40286400
H	-4.41447600	-2.12745200	2.86520900
H	-3.32168100	1.71243600	2.82347300
C	-4.29595500	1.71692300	0.87381000
H	-3.36864800	1.66881300	0.28654700
H	-5.03902100	1.11186100	0.34096300
C	-4.78777800	3.16940100	0.96130300
H	-5.70958700	3.20554800	1.55983200
H	-4.04585700	3.77706000	1.50020100
C	-5.05292500	3.79285200	-0.41647300
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H	-5.79583500	3.18348500	-0.95187500
C	-5.54810400	5.24357100	-0.33924700
H	-6.46711800	5.28078600	0.26470300
H	-4.80433600	5.85322000	0.19584600
C	-5.82046900	5.86839300	-1.71435300
H	-6.56478700	5.25900400	-2.24908300
H	-4.90186400	5.83041000	-2.31967300
C	-6.31619900	7.31914800	-1.64052100
H	-7.23393800	7.35710900	-1.03583900
H	-5.57236800	7.92876200	-1.10700900
C	-6.58715100	7.93496900	-3.01823200
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H	-6.93802200	8.97003400	-2.93074500
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C	4.75211700	-1.88868500	0.80288100
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C	5.84926500	-2.96205400	0.77756200
H	6.81258900	-2.51272400	1.06290200
H	5.62795100	-3.72627200	1.53708100
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C	7.07674700	-4.72118600	-0.63672100
H	6.85196200	-5.48874900	0.11923400
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H	7.44490700	-4.62239800	-2.76676500
H	6.24937700	-5.82703400	-2.30227300
C	8.29645300	-6.47989100	-2.05899600
H	8.06869200	-7.24756700	-1.30511100
H	9.26378000	-6.04415900	-1.76920000
C	8.42739600	-7.14095100	-3.43637200
H	8.68942500	-6.40380700	-4.20649100
H	9.20525900	-7.91391500	-3.43691900
H	7.48513600	-7.61592200	-3.73911600
H	3.11978000	1.80767600	2.66763800
C	4.29330200	1.74114400	0.84940000
H	5.12964000	1.15967000	0.44252100
H	3.44440500	1.58266000	0.16893600
C	4.67343200	3.22826900	0.87651200
H	3.83572500	3.81591000	1.28250900
H	5.51527700	3.37568400	1.56917300
C	5.05446400	3.77583300	-0.50635500
H	5.88952200	3.18476600	-0.91067200
H	4.21194800	3.62933400	-1.19927900
C	5.44600600	5.25974800	-0.49060400
H	4.61120700	5.85214800	-0.08567900
H	6.28855600	5.40460600	0.20229000
C	5.82918800	5.80415000	-1.87357900
H	4.98667500	5.65958000	-2.56733500
H	6.66342000	5.21125100	-2.27843600
C	6.22402900	7.28733000	-1.86271700
H	7.06617800	7.43210600	-1.17045800
H	5.39056000	7.88085300	-1.45912800
C	6.60606900	7.82069100	-3.24856200
H	6.88257000	8.88094600	-3.20657500
H	7.45994200	7.26971200	-3.66338000

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H	-1.09384900	-2.07412700	2.45709300

TODGA(-H)•



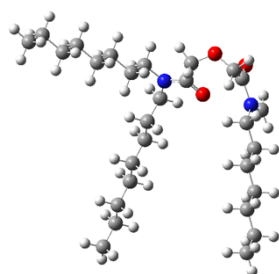
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H	-0.59131700	-1.97995100	-1.07859000
C	1.13969800	-0.13028400	-0.90488700
H	1.32415700	-0.91594200	-1.62768400
C	-2.10415000	-1.32168100	0.25370300
C	2.09378700	0.88474500	-0.48232200
N	-2.90661100	-0.31527600	0.68712600
N	3.34605000	0.87444600	-1.06960900
O	1.77968700	1.73712800	0.36938600
O	-2.20295800	-2.48295800	0.66923800
C	-2.82326700	1.07758700	0.22037500
H	-2.82319000	1.72167000	1.10900300
C	-3.88251600	-0.63588800	1.74350600
H	-4.14564300	0.30863300	2.23221000
C	3.78874900	-0.13593500	-2.03614900
H	4.59365800	0.31798400	-2.62513700
C	4.28873200	1.91955100	-0.65268200
H	4.95307300	2.11991300	-1.50201400
C	-5.15075500	-1.34840300	1.24994100
H	-5.66296700	-0.72090900	0.50837600
H	-4.85867200	-2.27509900	0.74249800
C	-6.11063000	-1.67014400	2.40376200
H	-5.59013900	-2.29549000	3.14427600
H	-6.38448500	-0.73962800	2.92496200

C	-7.38895700	-2.38737200	1.94733100
H	-7.90928000	-1.76426300	1.20388500
H	-7.11482000	-3.31835900	1.42888300
C	-8.35206300	-2.71258900	3.09741600
H	-8.62506900	-1.78090200	3.61638800
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C	-9.63026900	-3.43126200	2.64388900
H	-9.35809300	-4.36351400	2.12555600
H	-10.15237300	-2.80970900	1.90007200
C	-10.59394800	-3.75703000	3.79336300
H	-10.86689400	-2.82584900	4.31133300
H	-10.07319100	-4.37863900	4.53641000
C	-11.86774700	-4.47518200	3.33143200
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H	-1.85636400	1.23438000	-0.25823500
C	-3.96123200	1.49304000	-0.72377300
H	-3.98110200	0.81219600	-1.58695800
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C	-4.93876300	3.38991600	-2.14486600
H	-4.97682700	2.71603300	-3.01428500
H	-5.90422800	3.27742600	-1.62854900
C	-4.79199400	4.83775300	-2.63303700
H	-4.75322000	5.51124400	-1.76342200
H	-3.82649600	4.95010100	-3.14937800
C	-5.92195000	5.28609900	-3.57008600
H	-6.88780800	5.17536200	-3.05349200
H	-5.96196500	4.61193700	-4.43955700
C	-5.77656900	6.73306700	-4.06127500
H	-5.73762200	7.40741500	-3.19329400
H	-4.81205400	6.84428400	-4.57806200
C	-6.90953900	7.17172300	-4.99697700
H	-7.88461900	7.10519800	-4.49701100
H	-6.77573700	8.20832800	-5.32942900
H	-6.95234100	6.53740400	-5.89196700
H	3.70820300	2.82584200	-0.45835900
C	5.11806900	1.57663000	0.59561000
H	5.72764000	0.68302700	0.40300100
H	4.43035700	1.32623200	1.41290400

C	6.02945100	2.73611100	1.02012300
H	6.70203000	2.99878200	0.18857600
H	5.41423400	3.62785500	1.21148100
C	6.86776000	2.42345300	2.26763000
H	7.48033100	1.52857500	2.07850800
H	6.19468500	2.16366100	3.09830900
C	7.78146000	3.57918000	2.69844000
H	7.16868800	4.47345700	2.88872000
H	8.45326700	3.84029900	1.86623300
C	8.62005200	3.26663600	3.94542600
H	9.23310400	2.37189800	3.75624600
H	7.94885200	3.00601200	4.77809300
C	9.53442000	4.42108800	4.37824100
H	8.92251000	5.31507500	4.56822400
H	10.20628000	4.68158800	3.54714200
C	10.36738600	4.09966100	5.62506000
H	11.01588800	3.23028300	5.45508400
H	11.00868200	4.94362100	5.90724200
H	9.72288600	3.86907700	6.48329400
H	2.97991900	-0.33778100	-2.74899000
C	4.28995500	-1.45623400	-1.42453000
H	5.14152800	-1.24723800	-0.76445500
H	3.50459500	-1.88503200	-0.78723900
C	4.70376000	-2.47480700	-2.49528500
H	3.84389300	-2.68987300	-3.14834500
H	5.47533600	-2.03127100	-3.14314700
C	5.23333200	-3.79068200	-1.90771600
H	6.09684800	-3.57562900	-1.26046300
H	4.46458900	-4.23105500	-1.25512200
C	5.64203300	-4.81722500	-2.97312000
H	4.77738800	-5.03329300	-3.61920200
H	6.40957300	-4.37558600	-3.62704100
C	6.17416600	-6.13145200	-2.38529300
H	5.40735300	-6.57310000	-1.73059600
H	7.03945200	-5.91633400	-1.73965400
C	6.58240200	-7.16059300	-3.44842900
H	7.34932400	-6.72029100	-4.10253400
H	5.71795500	-7.37671700	-4.09329000
C	7.11247400	-8.46988800	-2.85147800
H	7.39487600	-9.18240900	-3.63605600
H	7.99856500	-8.29118000	-2.22856700
H	6.35541600	-8.95227800	-2.21966200

TODGA^{•+} degradation products

DPX cation



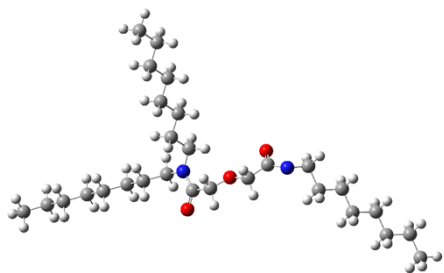
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O	2.26702300	-3.84783200	1.87394500
C	3.39386800	-3.25693100	1.27155600
H	4.18496700	-4.01816800	1.26722500
H	3.19326700	-2.95190700	0.24234800
C	0.99522800	-3.34580600	1.48359700
H	0.28210700	-4.00819300	1.97122200
H	0.86614100	-3.44423400	0.39465800
C	3.89694200	-2.10932700	2.14136500
C	0.79652800	-1.87040200	1.85199600
N	4.50072700	-0.87270100	1.42582200
N	-0.41323600	-1.43406900	2.24682400
O	1.78152900	-1.10321200	1.73204600
O	4.01972300	-2.15016100	3.32791300
C	5.10593300	-0.03761800	2.18342500
H	5.55029300	0.86036000	1.77228700
C	-1.60186100	-2.30573200	2.37927400
H	-2.30821300	-1.75838300	3.00926100
C	-0.57668900	0.00083600	2.56488700
H	-1.20252200	0.06283100	3.46178500
C	4.33630100	-0.69395000	-0.04601900
H	4.83332900	-1.54915800	-0.51782000
H	3.26073500	-0.77426600	-0.22165300
C	4.87951500	0.61846500	-0.60495800
H	4.42162600	1.46600300	-0.07764300
H	5.96638800	0.68043400	-0.45698400
C	4.56315400	0.74113300	-2.10649100
H	5.00357200	-0.10899500	-2.64649800
H	3.47572700	0.67431100	-2.25176700
C	5.07844100	2.05469400	-2.71356900
H	6.16820300	2.11609100	-2.57742600
H	4.64936700	2.90292900	-2.15944100
C	4.74258800	2.20057300	-4.20458900

H	3.65229000	2.13575500	-4.33952900
H	5.17100200	1.35225000	-4.75973100
C	5.24970400	3.51265200	-4.82045500
H	6.33925000	3.57774700	-4.68732700
H	4.82164200	4.36292600	-4.26935900
C	4.90866100	3.64589700	-6.30930700
H	3.82346600	3.61974100	-6.47149100
H	5.28451900	4.58964500	-6.72123200
H	5.35117100	2.82765700	-6.89176600
H	5.15361400	-0.25491000	3.24697100
H	0.41078700	0.38928200	2.81839700
C	-1.18954500	0.82576500	1.42497100
H	-2.20191600	0.46352700	1.20254500
H	-0.59164100	0.67679400	0.51559900
C	-1.24693000	2.32111000	1.76916200
H	-1.84228300	2.46354200	2.68318300
H	-0.23289700	2.67739400	2.00484900
C	-1.83644700	3.17984500	0.64127300
H	-2.85200600	2.82654800	0.40844400
H	-1.24337500	3.03212400	-0.27416800
C	-1.88525300	4.67707600	0.97592100
H	-0.86958000	5.02867500	1.21358100
H	-2.48137500	4.82514500	1.88892600
C	-2.46691400	5.53856700	-0.15343400
H	-3.48335400	5.18911800	-0.39031900
H	-1.87191600	5.38955100	-1.06774100
C	-2.51365900	7.03652500	0.17834800
H	-1.49804600	7.38669300	0.41443400
H	-3.10854800	7.18603900	1.09105800
C	-3.09627000	7.88935100	-0.95494700
H	-4.12507400	7.58736700	-1.18961900
H	-3.11442900	8.95227500	-0.68623500
H	-2.50329100	7.78765600	-1.87317300
H	-1.32913300	-3.20442900	2.94280500
C	-2.28625600	-2.68668600	1.05795700
H	-2.58012800	-1.77407700	0.52430000
H	-1.57842000	-3.21427100	0.40431200
C	-3.51726100	-3.57400900	1.29391800
H	-3.21237600	-4.48468000	1.83096100
H	-4.22206600	-3.04909600	1.95557600
C	-4.23771000	-3.96825700	-0.00324100
H	-4.54899000	-3.05752300	-0.53640300
H	-3.53109300	-4.48763600	-0.66820100
C	-5.46286700	-4.86285500	0.23116500

H	-5.14923900	-5.77468500	0.76164700
H	-6.16615300	-4.34550700	0.90108400
C	-6.19143100	-5.25474500	-1.06166000
H	-5.48778100	-5.76906200	-1.73418900
H	-6.50917600	-4.34308200	-1.59037800
C	-7.41338500	-6.15400400	-0.82825200
H	-8.11630400	-5.64133000	-0.15552100
H	-7.09572300	-7.06579300	-0.30163600
C	-8.13715000	-6.53943500	-2.12389700
H	-9.00233200	-7.18211600	-1.92203500
H	-8.49960200	-5.65000300	-2.65534700
H	-7.46949300	-7.08356300	-2.80448100

DPX radical



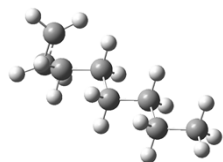
O 2

O	-1.09789600	0.05911100	-0.63816700
C	-2.16396000	0.74182900	-1.25091600
H	-1.80769600	1.60135600	-1.84498200
H	-2.72111500	0.08533300	-1.93961900
C	-0.11545400	-0.37770100	-1.57352400
H	0.38339400	0.49135000	-2.03365300
H	-0.57601700	-0.97653700	-2.36729300
C	-3.11613200	1.27550900	-0.19045400
C	0.89651600	-1.29790700	-0.87824800
N	-4.30266100	1.74966700	-0.72569700
N	1.71523100	-0.77639600	0.07476900
O	0.95114700	-2.48569000	-1.22169300
O	-2.82179100	1.39567200	0.99570500
C	-5.49614900	1.66337100	0.07566000
H	-6.03753100	2.61293600	-0.01807100
C	1.68562300	0.62547000	0.51696100
H	1.68955500	0.62379400	1.61483300
C	2.64898900	-1.69735800	0.74425300
H	2.91783200	-1.24023600	1.70313900
C	-6.40823200	0.52694400	-0.46397900

H	-6.59471300	0.69727500	-1.53154400
H	-5.87500200	-0.42868200	-0.37644800
C	-7.73685600	0.45735700	0.30142700
H	-7.53487300	0.30398900	1.37127800
H	-8.25534500	1.42371200	0.21796200
C	-8.65802000	-0.66014600	-0.20853000
H	-8.85533900	-0.50754500	-1.28020200
H	-8.13731000	-1.62583800	-0.12596900
C	-9.99253900	-0.73806200	0.54663100
H	-10.51302200	0.22816900	0.46365600
H	-9.79404900	-0.88805400	1.61866700
C	-10.91639400	-1.85521100	0.04215700
H	-10.39660700	-2.82190700	0.12590400
H	-11.11420600	-1.70657400	-1.03051300
C	-12.25198200	-1.93427000	0.79457300
H	-12.77213100	-0.96877800	0.71064400
H	-12.05495100	-2.08334500	1.86630700
C	-13.16867000	-3.05285600	0.28464400
H	-12.69003700	-4.03535200	0.38787500
H	-14.11281500	-3.08199200	0.84202600
H	-13.41210600	-2.91281200	-0.77660600
H	-5.25759900	1.47837600	1.13094400
H	2.10798000	-2.62582100	0.95558100
C	3.91641900	-2.02253300	-0.06074600
H	4.47260600	-1.09786200	-0.26510000
H	3.61913100	-2.44088400	-1.02936600
C	4.82380000	-3.01728200	0.67631300
H	5.09961400	-2.60550400	1.65969000
H	4.26058700	-3.94085100	0.87679600
C	6.10129600	-3.36401400	-0.10117200
H	6.66541500	-2.44055400	-0.30298900
H	5.82512900	-3.77516200	-1.08370000
C	7.01061800	-4.36257600	0.62835200
H	6.44651800	-5.28625500	0.82841500
H	7.28423000	-3.95226400	1.61260100
C	8.28895700	-4.70928700	-0.14721100
H	8.85453800	-3.78605100	-0.34704300
H	8.01620900	-5.11920000	-1.13179900
C	9.19837900	-5.70930500	0.58019400
H	8.63438200	-6.63243100	0.77885200
H	9.47158000	-5.30040400	1.56411600
C	10.47294700	-6.04940600	-0.20177100
H	11.07644800	-5.15100500	-0.38596000
H	11.09928200	-6.76527200	0.34446600

H	10.23291100	-6.49266900	-1.17698400
H	0.73168500	1.06368100	0.22260700
C	2.85321300	1.47710100	-0.00377300
H	3.80671700	1.04896500	0.33285700
H	2.86525200	1.43866100	-1.10250300
C	2.75703000	2.93555800	0.46620800
H	1.80440600	3.36761400	0.12450400
H	2.72610300	2.96214500	1.56589500
C	3.91712500	3.81114200	-0.02799600
H	4.86920400	3.37787400	0.31421300
H	3.94777300	3.78593200	-1.12790500
C	3.82703000	5.26937600	0.44277400
H	2.87489000	5.70277600	0.10053000
H	3.79548500	5.29354700	1.54272000
C	4.98717400	6.14579700	-0.04899600
H	5.01920100	6.12256400	-1.14920500
H	5.93982700	5.71295000	0.29315300
C	4.89889000	7.60420900	0.42154300
H	4.86796700	7.62823100	1.52072000
H	3.94754200	8.03752800	0.07959500
C	6.06163100	8.47227100	-0.07452800
H	5.96851400	9.50644800	0.27874100
H	7.02531700	8.08423400	0.28028500
H	6.09810000	8.49664800	-1.17145400

OCT cation

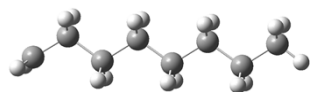


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C	-3.68037000	-0.32748100	-0.68009400
H	-3.36603200	-0.19957500	-1.71296000
H	-4.25886100	-1.21620000	-0.43941300
C	-3.43593800	0.66115500	0.27318200
H	-3.08321600	1.63533800	-0.05154400
H	-3.96278400	0.63727900	1.22186100
C	-2.09238000	-0.38573500	0.35199800
H	-2.20620900	-0.78126600	1.36323400
H	-2.08300500	-1.29622900	-0.28018400
C	-0.81774500	0.41199900	0.03816200

H	-0.86744800	0.78610100	-0.99215600
H	-0.77166200	1.28416400	0.69857800
C	0.43897200	-0.45467700	0.22020700
H	0.48273400	-0.82521500	1.25391400
H	0.37633600	-1.33888800	-0.43058900
C	1.72296000	0.32762800	-0.09759100
H	1.75807200	1.23557800	0.52193100
H	1.69042100	0.66646200	-1.14347600
C	3.00091600	-0.49138600	0.13374800
H	2.95892300	-1.41027900	-0.46835700
H	3.03914200	-0.81165200	1.18447800
C	4.27612700	0.28694000	-0.21065300
H	5.17014500	-0.31906800	-0.02568100
H	4.28723000	0.58388500	-1.26693200
H	4.36096000	1.19891000	0.39354200

OCT radical

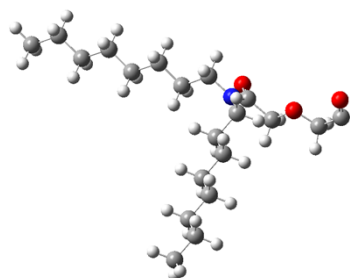


O 2

C	-4.55642500	-0.23058500	-0.00010400
H	-4.99354300	-0.58827900	-0.92864300
H	-4.99641500	-0.58400400	0.92870800
C	-3.27366200	0.53312800	-0.00005500
H	-3.22577200	1.18730700	-0.88290900
H	-3.22604400	1.18769500	0.88248400
C	-2.01129800	-0.37102500	0.00018300
H	-2.04269000	-1.02851300	0.88052900
H	-2.04275200	-1.02904800	-0.87976800
C	-0.70160200	0.42951000	-0.00013900
H	-0.68058600	1.09004300	-0.88027900
H	-0.68053800	1.09066500	0.87953100
C	0.55384200	-0.45409500	0.00012300
H	0.53180500	-1.11486800	0.88006400
H	0.53180700	-1.11541100	-0.87941300
C	1.86558900	0.34335500	-0.00013900
H	1.88862400	1.00498400	0.87939800
H	1.88866100	1.00437400	-0.88013700
C	3.12183800	-0.53877600	0.00020200
H	3.09987600	-1.19958100	-0.87875100
H	3.09986600	-1.19893400	0.87963600

C	4.42730600	0.26592000	-0.00007300
H	5.30407400	-0.39307600	0.00022000
H	4.49507200	0.91067500	-0.88594600
H	4.49502800	0.91138600	0.88528500

DPIX radical

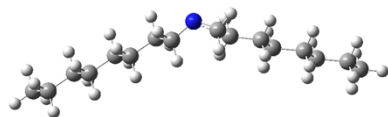


O 2

O	-2.41415600	-3.82597300	-0.27593900
C	-3.57821300	-4.38716000	-0.84744000
H	-4.13191100	-3.65559900	-1.45980800
H	-3.34148800	-5.24408900	-1.49840300
C	-1.52566700	-3.29292800	-1.26150500
H	-1.98564700	-2.42192900	-1.75532200
H	-1.29808900	-4.04882000	-2.02102600
C	-4.53862200	-4.88283000	0.20928800
C	-0.18572800	-2.92832800	-0.60817800
N	-0.14306500	-1.89019700	0.26970300
O	0.81915300	-3.58033100	-0.91617200
O	-4.44654300	-4.83814100	1.39177200
C	-1.31221100	-1.09500100	0.67111400
H	-1.29339800	-1.01294700	1.76577000
C	1.15425400	-1.58557300	0.89745900
H	0.94218600	-1.03596600	1.82138300
H	1.62281000	-2.53620400	1.17299100
C	2.11928600	-0.78266800	0.01193000
H	1.66040100	0.17730500	-0.26002300
H	2.28373700	-1.33671300	-0.91954700
C	3.46390000	-0.53153900	0.70833600
H	3.29435400	0.00627100	1.65416300
H	3.91691400	-1.49651800	0.98010700
C	4.45255100	0.26491100	-0.15488800
H	3.99942200	1.22990000	-0.42917600
H	4.62128900	-0.27368800	-1.09939500
C	5.80179000	0.51726700	0.53203900
H	6.25468900	-0.44778300	0.80577300

H	5.63285200	1.05494100	1.47771100
C	6.79054300	1.31254500	-0.33161600
H	6.33847800	2.27828700	-0.60580300
H	6.95964600	0.77533400	-1.27747000
C	8.14126700	1.56509400	0.35237600
H	8.59405600	0.60067300	0.62543700
H	7.97341000	2.10239400	1.29738800
C	9.12200900	2.35995200	-0.51827600
H	8.71204200	3.34433100	-0.77942300
H	10.07566100	2.52268800	-0.00140900
H	9.33703800	1.83147800	-1.45615300
H	-2.21578200	-1.65547300	0.42866900
C	-1.36846900	0.30789100	0.04800700
H	-0.47525700	0.87847700	0.33443400
H	-1.34196900	0.21716400	-1.04732600
C	-2.62407500	1.07976300	0.47793600
H	-3.52039000	0.51214300	0.18505900
H	-2.65159900	1.14755000	1.57594500
C	-2.70253800	2.49251300	-0.11759200
H	-1.80682900	3.05974600	0.17743100
H	-2.67389500	2.42548500	-1.21575900
C	-3.95614400	3.26826000	0.31000000
H	-4.85207900	2.70130600	0.01419500
H	-3.98481200	3.33335800	1.40834700
C	-4.03424800	4.68203300	-0.28243000
H	-4.00499200	4.61784200	-1.38107300
H	-3.13897700	5.24994500	0.01397100
C	-5.28756600	5.45920800	0.14343100
H	-5.31693000	5.52458300	1.24095300
H	-6.18253800	4.89270300	-0.15301100
C	-5.35695300	6.87017000	-0.45310100
H	-6.26269600	7.39747500	-0.12984600
H	-4.49256900	7.47316900	-0.14595700
H	-5.36432000	6.83664500	-1.55035700

DPH cation



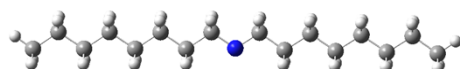
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N	-0.17905700	-2.92018200	-0.46887500
C	-1.34934400	-3.07351200	0.17616200

H	-1.35918500	-3.13056900	1.27056000
C	0.97145200	-2.52126600	0.25337100
H	0.78426800	-2.31889300	1.31801500
H	1.58025900	-3.45126600	0.18758700
C	1.79446900	-1.41253400	-0.45054400
H	1.19508900	-0.49357400	-0.46301400
H	1.96481800	-1.70610100	-1.49201500
C	3.12362200	-1.16338000	0.27430900
H	2.93034200	-0.93147000	1.33144900
H	3.72358300	-2.08438600	0.26087900
C	3.92742600	-0.01807100	-0.35822300
H	3.32410100	0.90173600	-0.34459300
H	4.11702200	-0.24857900	-1.41654200
C	5.26197800	0.23935100	0.35671100
H	5.86623300	-0.67976700	0.33768800
H	5.06803600	0.45812100	1.41747600
C	6.06956400	1.39046400	-0.25832200
H	5.46436900	2.30962200	-0.24020800
H	6.26450600	1.17253300	-1.31926600
C	7.40260900	1.64953200	0.45754600
H	8.00845300	0.73205200	0.43670300
H	7.20751300	1.86381100	1.51840800
C	8.20314400	2.80363200	-0.15708200
H	7.63769000	3.74360200	-0.11824300
H	9.14808600	2.96118800	0.37611600
H	8.44320400	2.60364300	-1.20922200
H	-2.07296400	-3.69651700	-0.34952200
C	-1.83500500	-1.45431000	-0.20747900
H	-1.23563000	-0.81195400	0.43834900
H	-1.63311200	-1.25578400	-1.25901700
C	-3.33261700	-1.41953600	0.11183300
H	-3.88160500	-2.08714100	-0.55922800
H	-3.51967300	-1.73584300	1.14308400
C	-3.80559500	0.04008300	-0.09340000
H	-3.26766600	0.70424200	0.59503400
H	-3.56710100	0.36695900	-1.11365500
C	-5.32340400	0.16535600	0.14632400
H	-5.85612400	-0.50982100	-0.53729900
H	-5.56017300	-0.16621500	1.16671300
C	-5.82401600	1.60362700	-0.05932000
H	-5.58143800	1.93169400	-1.08063500
H	-5.28509200	2.27937500	0.62069700
C	-7.33579900	1.74849400	0.17277100
H	-7.57926400	1.42117600	1.19348300

H	-7.87273900	1.07026800	-0.50557300
C	-7.83406200	3.18328200	-0.03841100
H	-8.91412600	3.25538700	0.13422800
H	-7.33862800	3.88119700	0.64832100
H	-7.63617300	3.52526700	-1.06211100

DPIII radical

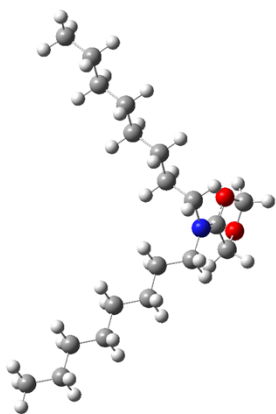


O 2

N	0.00001600	0.31255200	-0.00069300
C	-1.20494900	-0.48360200	-0.01193100
H	-1.20275200	-1.17359500	0.85431300
C	1.20494000	-0.48367200	0.01110900
H	1.20261300	-1.13870700	0.90420900
H	1.20276900	-1.17407400	-0.85480700
C	2.47178800	0.37566000	-0.00473800
H	2.44912700	1.05095600	0.86160400
H	2.45163300	1.01549000	-0.89770300
C	3.76129200	-0.45508000	0.01349100
H	3.76993900	-1.09809800	0.90718700
H	3.77056600	-1.13566100	-0.85195000
C	5.03665000	0.39902500	-0.00452900
H	5.02949800	1.07824200	0.86138200
H	5.02852400	1.04240600	-0.89738700
C	6.32944300	-0.42830200	0.01145700
H	6.33571100	-1.10764400	-0.85475400
H	6.33694400	-1.07196600	0.90448500
C	7.60527900	0.42481200	-0.00677600
H	7.60032100	1.10406100	0.85956100
H	7.59858300	1.06903300	-0.89946000
C	8.89886100	-0.40135700	0.00837100
H	8.90489200	-1.07960900	-0.85755500
H	8.90660400	-1.04473500	0.90050000
C	10.16797800	0.45928800	-0.00994600
H	10.20832200	1.12429900	0.86257500
H	11.07281200	-0.16058700	0.00148400
H	10.20660200	1.08913600	-0.90825900
H	-1.20277800	-1.13906000	-0.90472100
C	-2.47177000	0.37578600	0.00369900
H	-2.45142500	1.01599200	0.89639100
H	-2.44925200	1.05072000	-0.86292800

C	-3.76128700	-0.45494500	-0.01392500
H	-3.77014500	-1.09829500	-0.90738200
H	-3.77036100	-1.13521000	0.85176800
C	-5.03665600	0.39914400	0.00409500
H	-5.02829300	1.04288900	0.89668900
H	-5.02977200	1.07800900	-0.86209400
C	-6.32942800	-0.42823300	-0.01117700
H	-6.33718300	-1.07223800	-0.90395700
H	-6.33539400	-1.10724400	0.85529500
C	-7.60529700	0.42482700	0.00714100
H	-7.60067900	1.10371600	-0.85948000
H	-7.59832300	1.06942000	0.89955600
C	-8.89884100	-0.40141800	-0.00720300
H	-8.90451900	-1.07932200	0.85899900
H	-8.90687100	-1.04515500	-0.89907100
C	-10.16800100	0.45916000	0.01123200
H	-11.07280300	-0.16077200	0.00037900
H	-10.20633400	1.08936500	0.90930600
H	-10.20870200	1.12382000	-0.86154100

DPVIII cation

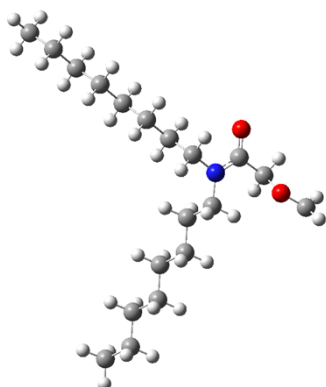


1 1			
O	-0.32695900	-5.38506900	-1.44014900
C	-1.39227500	-5.39504900	-0.49880700
H	-1.51635800	-6.38068100	-0.02342600
H	-2.31287300	-5.10786600	-1.00861100
C	-0.90457000	-4.38067700	0.51947600
N	-1.56124800	-3.79390200	1.47150000
O	0.37885800	-4.16233200	0.33958200
C	-3.00936400	-4.06705100	1.68624300

H	-3.12308000	-4.28050700	2.75331100
C	-0.86770300	-2.84329400	2.39443100
H	-1.52093800	-2.74423400	3.26420100
H	0.05739800	-3.32716100	2.72097100
C	-0.57028200	-1.47333500	1.77112300
H	-1.50342300	-1.01210600	1.42690800
H	0.07235100	-1.60042500	0.89201500
C	0.12251300	-0.54972200	2.78560500
H	-0.52023700	-0.42944500	3.66985100
H	1.05009700	-1.02414500	3.13725000
C	0.44889000	0.83305000	2.20324600
H	-0.47887000	1.30493100	1.84732600
H	1.09218800	0.71178200	1.31914700
C	1.13906600	1.76455300	3.20931500
H	2.06593300	1.29044600	3.56573600
H	0.49532700	1.88378900	4.09376800
C	1.46784600	3.14825300	2.63223000
H	0.54089400	3.62311500	2.27626400
H	2.11061200	3.02951800	1.74662900
C	2.15971800	4.08151800	3.63550100
H	3.08593400	3.60709300	3.99118800
H	1.51754500	4.20135400	4.52021000
C	2.48539300	5.46104400	3.05102300
H	1.57480600	5.97598100	2.71876700
H	2.97896800	6.10170000	3.79131700
H	3.15399900	5.37679100	2.18460300
H	-3.27007100	-4.98148700	1.14779100
C	-3.91519400	-2.90898300	1.25753000
H	-3.64825000	-2.00317400	1.81480100
H	-3.74747900	-2.69329100	0.19388800
C	-5.39611400	-3.23944800	1.50137900
H	-5.66884000	-4.14410600	0.93862100
H	-5.54492500	-3.47789000	2.56440600
C	-6.33319600	-2.09048800	1.10231100
H	-6.05536800	-1.18548100	1.66259900
H	-6.18344600	-1.85306700	0.03865600
C	-7.81470200	-2.40609600	1.35025100
H	-8.09310000	-3.30951100	0.78702100
H	-7.95978800	-2.65006400	2.41335300
C	-8.75529900	-1.25715100	0.96189000
H	-8.61183900	-1.01360500	-0.10187500
H	-8.47536600	-0.35293900	1.52359100
C	-10.23723500	-1.56831900	1.21326400
H	-10.37962100	-1.81399600	2.27568100

H	-10.51834400	-2.47006900	0.64998000
C	-11.17017200	-0.41448600	0.82729700
H	-12.21926800	-0.66855800	1.01942200
H	-10.93676600	0.49255300	1.39959700
H	-11.07650500	-0.16820700	-0.23821900
C	0.83178900	-5.07567700	-0.73135200
H	1.28022900	-5.93983500	-0.22841400
H	1.53529300	-4.53719000	-1.36249100

DPVIII radical

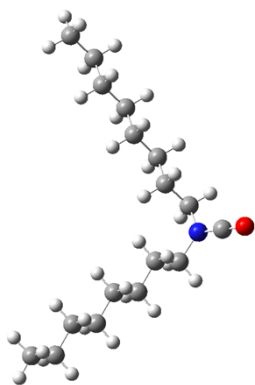


O 2

O	1.92875400	4.69271900	0.02943400
C	1.17485300	4.04889500	-1.00508300
H	1.81134800	3.31683500	-1.52150900
H	0.82652500	4.79337500	-1.72727600
C	-0.07653300	3.39921100	-0.40377700
N	0.07263600	2.32619000	0.41969500
O	-1.18601300	3.85891400	-0.69988700
C	1.36733300	1.74726600	0.80595500
H	1.36739400	1.63854800	1.89892900
C	-1.14744100	1.74860000	1.00892300
H	-0.83953500	1.19338000	1.90206500
H	-1.78629500	2.57716300	1.33270200
C	-1.94328900	0.83398400	0.06543600
H	-1.31025200	-0.00221000	-0.26024800
H	-2.21195100	1.40372400	-0.83155500
C	-3.21375400	0.28917400	0.73263700
H	-2.94272900	-0.26030100	1.64769000
H	-3.84349800	1.13169500	1.05503000
C	-4.03241900	-0.63105100	-0.18382600
H	-3.40251900	-1.47336800	-0.50854300
H	-4.30379900	-0.08146700	-1.09754500

C	-5.30603600	-1.17730900	0.47611800
H	-5.93688800	-0.33476100	0.79789000
H	-5.03434600	-1.72327100	1.39268300
C	-6.12369900	-2.10048900	-0.43776000
H	-5.49372000	-2.94419200	-0.75942000
H	-6.39537400	-1.55555800	-1.35483500
C	-7.39860900	-2.64623500	0.22016900
H	-8.02933200	-1.80385200	0.53999300
H	-7.12800800	-3.19067900	1.13685000
C	-8.20826400	-3.56825800	-0.69963100
H	-7.61568700	-4.43913300	-1.00895500
H	-9.11127100	-3.94008200	-0.20020800
H	-8.52346700	-3.04203800	-1.61004700
H	2.15664500	2.46324300	0.57511200
C	1.67301400	0.39195900	0.15125800
H	0.89966900	-0.33727800	0.42652300
H	1.62416000	0.50154500	-0.94142500
C	3.05062200	-0.14885900	0.55997600
H	3.82652000	0.57880900	0.27825500
H	3.09732000	-0.23707200	1.65600400
C	3.37895100	-1.50933700	-0.07079900
H	2.60308400	-2.23665100	0.21255600
H	3.33024000	-1.42157300	-1.16671600
C	4.75566500	-2.05546000	0.33255300
H	5.53161100	-1.32842900	0.04827600
H	4.80458800	-2.14176300	1.42878900
C	5.08321600	-3.41652700	-0.29667700
H	5.03370400	-3.33101800	-1.39310300
H	4.30784900	-4.14436400	-0.01203200
C	6.45988500	-3.96468600	0.10405000
H	6.50989300	-4.05122800	1.19940000
H	7.23519400	-3.23842500	-0.18087600
C	6.77806000	-5.32442700	-0.52947100
H	7.76690100	-5.68718000	-0.22359500
H	6.03948500	-6.08136500	-0.23503400
H	6.76996900	-5.26251200	-1.62546800
C	2.97934600	5.44393300	-0.40334200
H	2.92470700	5.86710400	-1.40488300
H	3.48609500	5.96565200	0.40002700

DPV cation

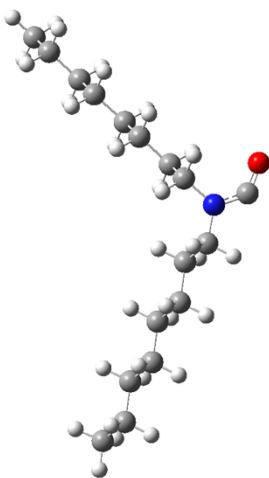


1 1

C	-0.03865200	3.91585600	-0.72907100
N	0.00642000	3.04936500	0.18317300
O	-0.06761700	4.71816100	-1.55308300
C	1.38128200	2.59630500	0.68602200
H	1.24851900	2.50048300	1.76656600
C	-1.29835100	2.49039000	0.75636300
H	-1.03839500	2.23573300	1.78619400
H	-2.00671000	3.32214400	0.78288800
C	-1.85108900	1.30366600	-0.02590900
H	-1.12690500	0.48186900	-0.02840000
H	-2.01726100	1.59375500	-1.07173600
C	-3.17694300	0.82834800	0.59532300
H	-3.00849100	0.53940300	1.64252800
H	-3.89333700	1.66209300	0.61171400
C	-3.79014200	-0.35497000	-0.16786100
H	-3.07436200	-1.18982400	-0.17949500
H	-3.94680000	-0.06658800	-1.21752600
C	-5.11951800	-0.83175500	0.43299800
H	-5.83160000	0.00687400	0.44944300
H	-4.96059600	-1.12113200	1.48258000
C	-5.74162200	-2.00959200	-0.32944500
H	-5.03055500	-2.84947700	-0.34428800
H	-5.89671800	-1.72078300	-1.38007400
C	-7.07411200	-2.48655600	0.26465400
H	-7.78401000	-1.64682000	0.28025600
H	-6.91897100	-2.77640300	1.31407500
C	-7.69043500	-3.66151500	-0.50356800
H	-7.01912400	-4.52986200	-0.50589300
H	-8.64032900	-3.97624200	-0.05578900
H	-7.88805700	-3.39181400	-1.54898100
H	2.06716600	3.42758400	0.50210300
C	1.86000900	1.31029100	0.02287700

H	1.15224000	0.49744700	0.22029800
H	1.89856500	1.45719500	-1.06434700
C	3.25577500	0.91796600	0.54110500
H	3.96069000	1.74126000	0.35727700
H	3.21649100	0.77390700	1.63002900
C	3.78143400	-0.36239900	-0.12570600
H	3.07006000	-1.18198000	0.05236100
H	3.81714700	-0.21376700	-1.21482800
C	5.17127200	-0.77798500	0.37577900
H	5.88155000	0.04400400	0.20142000
H	5.13466600	-0.92802000	1.46512200
C	5.69804200	-2.05430300	-0.29517200
H	5.73432000	-1.90317800	-1.38474800
H	4.98586800	-2.87558000	-0.12307200
C	7.08700700	-2.47903600	0.20122500
H	7.05129900	-2.63052600	1.28984400
H	7.79931000	-1.65911200	0.02878700
C	7.60416500	-3.75445600	-0.47466500
H	8.59694300	-4.02956500	-0.09972000
H	6.93164000	-4.60204900	-0.29028000
H	7.68301900	-3.62341000	-1.56155300

DPV radical

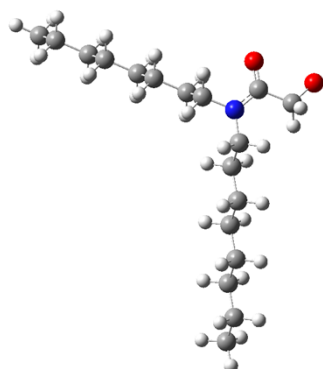


O 2			
C	-0.21399600	4.06120500	-0.76728800
N	0.01519000	3.08712700	0.11763900
O	-1.26068000	4.52074700	-1.17318600
C	1.39534300	2.73413300	0.47881100
H	1.49029400	2.79789900	1.57163900

C	-1.12072300	2.40641700	0.78330500
H	-0.72526600	1.94427700	1.69479300
H	-1.83656500	3.17896600	1.08703400
C	-1.82433600	1.36123500	-0.09134500
H	-1.10317900	0.59151600	-0.39599700
H	-2.17820800	1.84754400	-1.00909100
C	-3.00795800	0.70673200	0.63541200
H	-2.65244300	0.23306900	1.56347000
H	-3.72210600	1.48565600	0.94160500
C	-3.73792200	-0.34020600	-0.21794600
H	-3.02363600	-1.11847200	-0.52680800
H	-4.09419100	0.13393800	-1.14460900
C	-4.92253400	-0.99779000	0.50334000
H	-5.63702400	-0.21899900	0.81057700
H	-4.56561000	-1.46895900	1.43204600
C	-5.65301000	-2.04667000	-0.34654400
H	-4.93906900	-2.82603900	-0.65460300
H	-6.01089700	-1.57631500	-1.27518900
C	-6.83777900	-2.70521500	0.37368100
H	-7.55215300	-1.92719900	0.68039200
H	-6.48082500	-3.17549200	1.30176500
C	-7.56112700	-3.75204400	-0.48223000
H	-6.88097900	-4.56204200	-0.77632900
H	-8.40078800	-4.20268100	0.06083800
H	-7.96038700	-3.30466100	-1.40174500
H	2.04034700	3.50649200	0.04872700
C	1.83899100	1.34963600	-0.00881500
H	1.18994700	0.57595400	0.42411500
H	1.70785300	1.29907300	-1.09836600
C	3.29953300	1.04969400	0.35745700
H	3.94966000	1.82326700	-0.07798200
H	3.42532500	1.12128700	1.44850400
C	3.77090800	-0.33236400	-0.11614200
H	3.12176900	-1.10625500	0.32092500
H	3.64183000	-0.40436400	-1.20653400
C	5.23227700	-0.63632200	0.24181600
H	5.88086500	0.13834400	-0.19481100
H	5.36127300	-0.56406300	1.33259800
C	5.70476200	-2.01737100	-0.23277000
H	5.57563100	-2.09009800	-1.32357000
H	5.05673900	-2.79294500	0.20373900
C	7.16627400	-2.32348800	0.12290100
H	7.29594400	-2.25191900	1.21279900
H	7.81431300	-1.54936600	-0.31355400

C	7.62930100	-3.70480100	-0.35571900
H	8.67594100	-3.89184500	-0.08644400
H	7.02229400	-4.50301200	0.09099900
H	7.54438600	-3.79511700	-1.44645400

DPVII radical

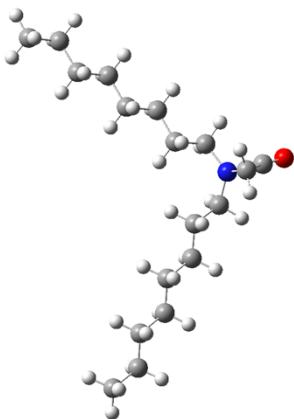


0 2

C	1.03431600	4.29105400	-0.78696100
H	1.78993600	3.58318100	-1.17093300
H	1.55648300	4.84823000	0.02129000
C	-0.21124700	3.58701700	-0.18401000
N	0.00627600	2.50732700	0.62368100
O	-1.33636700	4.00929100	-0.44072100
C	1.33583300	2.02036100	1.01628700
H	1.29590000	1.79081100	2.08874100
C	-1.17736700	1.82394700	1.17536100
H	-0.84370900	1.26587000	2.05729400
H	-1.88055800	2.59336000	1.51116800
C	-1.88716800	0.88297800	0.19077400
H	-1.18911400	0.10397600	-0.14441000
H	-2.17918900	1.45779700	-0.69580600
C	-3.12808700	0.23044900	0.81554900
H	-2.83542500	-0.32961700	1.71743000
H	-3.81945300	1.01703400	1.15255800
C	-3.86622100	-0.71154500	-0.14601200
H	-3.17521100	-1.49816600	-0.48576000
H	-4.15874200	-0.15086400	-1.04625300
C	-5.11079900	-1.36389800	0.47164400
H	-5.80186700	-0.57672800	0.80950500
H	-4.81804700	-1.92194400	1.37438000
C	-5.84968800	-2.30714000	-0.48762900
H	-5.15944700	-3.09536400	-0.82589800

H	-6.14258600	-1.74987200	-1.39059800
C	-7.09547900	-2.95898100	0.12820000
H	-7.78600700	-2.17195400	0.46501000
H	-6.80360700	-3.51622700	1.03057500
C	-7.82707600	-3.89959900	-0.83701100
H	-7.17283100	-4.71786100	-1.16513300
H	-8.71097200	-4.34777000	-0.36694500
H	-8.16236700	-3.36360200	-1.73442700
H	2.06271800	2.83024600	0.91365800
C	1.82320200	0.78556500	0.24273000
H	1.11489400	-0.04014200	0.39003000
H	1.82061600	1.00855300	-0.83353400
C	3.22627100	0.34439400	0.68207000
H	3.93430100	1.17308100	0.52861600
H	3.22253600	0.14143700	1.76374100
C	3.73415800	-0.89805200	-0.06311900
H	3.02791900	-1.72743500	0.09253500
H	3.73600800	-0.69635000	-1.14484000
C	5.13815000	-1.33935700	0.37274900
H	5.84384800	-0.50927800	0.21619500
H	5.13571400	-1.53861800	1.45528200
C	5.64828200	-2.58269300	-0.36871200
H	5.65028400	-2.38465300	-1.45154800
H	4.94384100	-3.41391200	-0.21164200
C	7.05293100	-3.02370400	0.06548300
H	7.05146700	-3.22184000	1.14739200
H	7.75735700	-2.19389000	-0.09242900
C	7.55467300	-4.26663000	-0.67942900
H	8.55915400	-4.55463300	-0.34633700
H	6.88953400	-5.12390300	-0.51282700
H	7.60058600	-4.08838600	-1.76163400
O	0.74061600	5.22610300	-1.73027700

DPVI cation

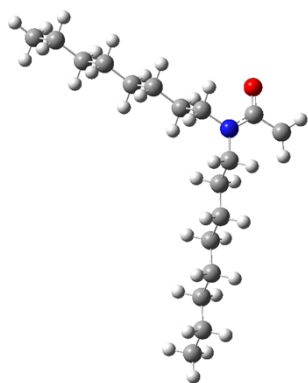


1 1

C	0.01217000	-4.36103100	-0.37638600
N	-0.00665600	-2.88904500	0.00034700
O	0.02907800	-5.40142200	0.17350000
C	-1.32164500	-2.37288800	0.54526300
H	-1.18564500	-2.34192900	1.62950200
C	1.29293900	-2.32752200	0.54095300
H	1.13513500	-2.23521700	1.61856200
H	2.04953400	-3.10450000	0.38564100
C	1.74883200	-1.01069900	-0.08549300
H	1.05417700	-0.20452700	0.17057400
H	1.75830800	-1.09130300	-1.18114000
C	3.16148100	-0.65170900	0.41231200
H	3.15850400	-0.60046400	1.51060700
H	3.85857000	-1.45751900	0.14080700
C	3.67799300	0.67801000	-0.15484800
H	2.98987200	1.48731600	0.12993700
H	3.66709200	0.63462600	-1.25414600
C	5.09486300	1.01989400	0.32773500
H	5.78116000	0.21005000	0.03765200
H	5.10518000	1.05159200	1.42758100
C	5.62340600	2.35187600	-0.22142500
H	4.93965900	3.16297800	0.07167200
H	5.61106900	2.32284300	-1.32168000
C	7.04195400	2.68916100	0.25885100
H	7.72551500	1.87975200	-0.03641000
H	7.05489500	2.71511700	1.35822700
C	7.56367200	4.02267400	-0.28880700
H	6.92051400	4.85685700	0.01968600
H	8.57723400	4.23277200	0.07239200
H	7.59551800	4.01576000	-1.38592300
H	-2.06631700	-3.14728700	0.33246400

C	-1.76928500	-1.02960700	-0.02704200
H	-1.08291800	-0.23560200	0.28375000
H	-1.74645400	-1.06222400	-1.12506300
C	-3.19523900	-0.68602400	0.44170100
H	-3.88420200	-1.48570500	0.13354500
H	-3.22182200	-0.65728300	1.54035500
C	-3.69075500	0.65600700	-0.11619700
H	-2.99832300	1.45415400	0.18918300
H	-3.66075900	0.62457000	-1.21558800
C	-5.11152800	1.01344400	0.34238800
H	-5.80314800	0.21279200	0.03981100
H	-5.14084000	1.04607000	1.44177300
C	-5.61002400	2.35257400	-0.21829300
H	-5.58088000	2.31942600	-1.31813800
H	-4.91668200	3.15269600	0.08253700
C	-7.02956900	2.71797400	0.23746400
H	-7.05960300	2.75076200	1.33626500
H	-7.72337800	1.91986100	-0.06450900
C	-7.51701400	4.05795000	-0.32621500
H	-8.53202200	4.28948400	0.01730300
H	-6.86308600	4.88167100	-0.01222000
H	-7.53132300	4.04516400	-1.42368900
C	-0.00047500	-3.41196700	-1.45858300
H	0.91950700	-3.21819200	-2.00759000
H	-0.92073300	-3.23858300	-2.01443300

DPVI radical



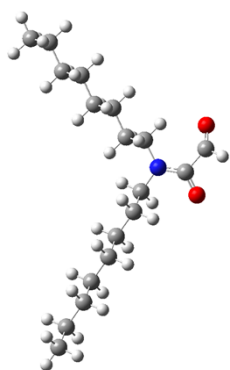
O 2			
C	0.12299100	-3.72934400	-0.58877900
N	0.00005200	-2.74757700	0.37013600
O	1.24517000	-4.13449800	-0.95842300
C	-1.28787200	-2.25146400	0.86769900

H	-1.13413800	-1.94341500	1.90849300
C	1.23983000	-2.18657400	0.92291000
H	1.01139600	-1.81303200	1.92758100
H	1.95713400	-3.00713200	1.02274800
C	1.87072200	-1.06910200	0.07596000
H	1.16725800	-0.22988300	-0.01268700
H	2.04353100	-1.45236000	-0.93700400
C	3.19318600	-0.57120300	0.67463900
H	3.02002800	-0.21186600	1.70109000
H	3.89258000	-1.41619400	0.75851400
C	3.84890300	0.54752800	-0.14716000
H	3.14874100	1.39253300	-0.23389400
H	4.02302800	0.18753100	-1.17217300
C	5.17331800	1.04736200	0.44629300
H	5.87377000	0.20258600	0.53049000
H	4.99918400	1.40360700	1.47332100
C	5.82931400	2.16788300	-0.37227800
H	5.12960500	3.01374200	-0.45664800
H	6.00378300	1.81257900	-1.39946000
C	7.15443700	2.66769400	0.21960400
H	7.85440200	1.82340000	0.30273000
H	6.98094300	3.02302700	1.24605100
C	7.80228000	3.78716300	-0.60429300
H	7.14012200	4.65983800	-0.67678800
H	8.74555000	4.12102300	-0.15496900
H	8.02034200	3.45125700	-1.62641500
H	-2.00153700	-3.08104200	0.90407600
C	-1.88576900	-1.07958700	0.07149400
H	-1.18162700	-0.23739000	0.08119400
H	-1.99832500	-1.37641100	-0.98053400
C	-3.24034200	-0.62624300	0.63289400
H	-3.94408400	-1.47256800	0.61820000
H	-3.12154700	-0.34636300	1.69074500
C	-3.85261100	0.55333200	-0.13573600
H	-3.15088000	1.40076800	-0.11695700
H	-3.96780900	0.27520400	-1.19421000
C	-5.20983900	1.00697000	0.41933500
H	-5.91118500	0.15881000	0.40025800
H	-5.09410300	1.28411100	1.47831200
C	-5.82284900	2.18670800	-0.34769000
H	-5.93888400	1.91033100	-1.40693300
H	-5.12221700	3.03559400	-0.32880100
C	-7.18035200	2.64146400	0.20588400
H	-7.06491800	2.91848400	1.26405100

H	-7.88108900	1.79389400	0.18646600
C	-7.78510400	3.82024500	-0.56632600
H	-8.75280000	4.12004400	-0.14606500
H	-7.12288600	4.69525800	-0.53603100
H	-7.94520300	3.56247100	-1.62132000
C	-1.07583900	-4.29749400	-1.19068300
H	-0.92509400	-5.11487100	-1.88553200
H	-2.08122100	-3.92658200	-1.03405200

TODGA(-H)[•] degradation products

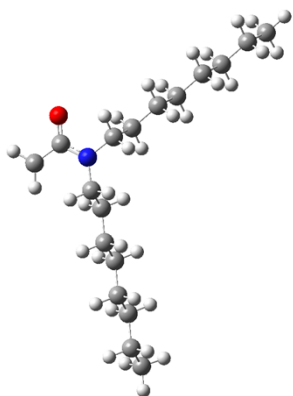
N,N-dioctyl-2-oxoacetamide



O 1			
O	-1.92626700	-4.86306000	-0.53212100
C	-0.89771600	-4.49454500	-1.06047000
H	-0.59768000	-4.85256500	-2.06329800
C	0.22134800	-3.66774100	-0.41274400
N	-0.02367600	-2.63489400	0.42239100
O	1.35519600	-4.06918800	-0.71285600
C	-1.36823700	-2.16168000	0.79680500
H	-1.38662700	-2.06974300	1.89054100
C	1.14477800	-1.95648300	1.01743200
H	0.78024600	-1.41354500	1.89586400
H	1.83836900	-2.72928700	1.36493300
C	1.87922600	-0.99919000	0.06668200
H	1.18573700	-0.22317800	-0.28292100
H	2.20826600	-1.55937500	-0.81607600
C	3.09105700	-0.34367000	0.74365200
H	2.76089600	0.20184000	1.64127300
H	3.77808900	-1.12770600	1.09505800
C	3.85251400	0.61772700	-0.17980000
H	3.16564400	1.40160600	-0.53372000
H	4.18238400	0.07154700	-1.07610300

C	5.06775000	1.27435700	0.48953200
H	5.75422900	0.48988900	0.84269100
H	4.73744900	1.81873200	1.38755800
C	5.83068900	2.23599700	-0.43193700
H	5.14494600	3.02136700	-0.78555900
H	6.16125200	1.69229400	-1.33019600
C	7.04702300	2.89261000	0.23550100
H	7.73302900	2.10847800	0.58795200
H	6.71745400	3.43645600	1.13301400
C	7.80297900	3.85145000	-0.69227900
H	7.15260600	4.66708200	-1.03430500
H	8.66492800	4.30267000	-0.18584200
H	8.17548700	3.32921100	-1.58311900
H	-2.09059400	-2.93322800	0.53472400
C	-1.76163700	-0.82481500	0.15264500
H	-1.04623800	-0.04291200	0.44031900
H	-1.69849400	-0.92206900	-0.94036400
C	-3.17857100	-0.39289600	0.55650600
H	-3.89394000	-1.17706800	0.26751500
H	-3.23683100	-0.31344300	1.65259600
C	-3.60818500	0.94099300	-0.07040000
H	-2.89355700	1.72585400	0.22047600
H	-3.54758200	0.86231200	-1.16635200
C	-5.02583200	1.37364000	0.32843800
H	-5.73931500	0.58747200	0.03827600
H	-5.08605300	1.45157000	1.42473500
C	-5.45998000	2.70612500	-0.29760600
H	-5.39968300	2.62906800	-1.39410400
H	-4.74750700	3.49356400	-0.00720900
C	-6.87821200	3.13844300	0.09959300
H	-6.93897600	3.21659300	1.19502300
H	-7.59036500	2.35216000	-0.19069500
C	-7.30453300	4.46983700	-0.53064500
H	-8.32078700	4.74922900	-0.22717100
H	-6.63145400	5.28370700	-0.23106100
H	-7.28780100	4.41269000	-1.62680800

N,N-dioctylacetamide radical



O 2

C	-1.07563300	-4.29751000	1.19096800
H	-2.08112300	-3.92699500	1.03419600
H	-0.92450700	-5.11461500	1.88605700
C	0.12305400	-3.72936500	0.58877900
N	0.00002400	-2.74746200	-0.37000200
O	1.24535500	-4.13460600	0.95813600
C	-1.28800500	-2.25159800	-0.86760200
H	-1.13441700	-1.94379700	-1.90849400
C	1.23969400	-2.18639800	-0.92297000
H	1.01102400	-1.81261400	-1.92752500
C	1.87082500	-1.06907900	-0.07604800
H	1.16738600	-0.22982200	0.01257400
H	2.04364500	-1.45234100	0.93690600
C	3.19330800	-0.57128500	-0.67469300
H	3.89270500	-1.41629800	-0.75839200
H	3.02028800	-0.21207300	-1.70121900
C	3.84892000	0.54755900	0.14704000
H	3.14875800	1.39260300	0.23348500
H	4.02280800	0.18773600	1.17216200
C	5.17347100	1.04725100	-0.44620700
H	4.99959600	1.40320600	-1.47338900
H	5.87395700	0.20245400	-0.53001100
C	5.82925600	2.16800100	0.37220500
H	6.00341900	1.81301300	1.39955800
H	5.12953000	3.01390300	0.45613000
C	7.15454800	2.66761700	-0.21944100
H	6.98136700	3.02260500	-1.24606600
H	7.85454500	1.82329100	-0.30208700
C	7.80215800	3.78735800	0.60426400
H	8.01992400	3.45180300	1.62656900
H	8.74556500	4.12106100	0.15510000

H	7.13998700	4.66007100	0.67627400
H	1.95687700	-3.00703100	-1.02325300
H	-2.00163600	-3.08119500	-0.90361700
C	-1.88582900	-1.07957200	-0.07152900
H	-1.99824300	-1.37621600	0.98056600
H	-1.18159500	-0.23745500	-0.08138400
C	-3.24046900	-0.62635900	-0.63282300
H	-3.12189600	-0.34675500	-1.69078000
H	-3.94419600	-1.47270100	-0.61778200
C	-3.85261100	0.55340300	0.13562000
H	-3.96753200	0.27555600	1.19420600
H	-3.15090300	1.40085700	0.11644900
C	-5.20998200	1.00685300	-0.41923000
H	-5.09452500	1.28367600	-1.47832900
H	-5.91131300	0.15867800	-0.39973700
C	-5.82283700	2.18679500	0.34759100
H	-5.12223400	3.03570700	0.32827900
H	-5.93858100	1.91073700	1.40695800
C	-7.18049400	2.64134200	-0.20575900
H	-7.06534800	2.91804600	-1.26404800
H	-7.88120200	1.79374900	-0.18591700
C	-7.78510100	3.82032700	0.56624500
H	-7.12293000	4.69536900	0.53552600
H	-8.75291800	4.11996100	0.14613500
H	-7.94492700	3.56286900	1.62136300