

**Revealing the Nature of Covalently Tethered Distonic Radical Anions in the
Generation of Heteroatom-Centered radicals: Evidence for the Polarity-
matching PCET Pathway**

Kang Fu¹, Xihui Yang¹, Zhiyou Yu¹, Lijuan Song^{1*}, Lei Shi^{1*}

Email: songlijuan@hit.edu.cn, lshi@hit.edu.cn

*¹School of Chemistry and Chemical Engineering, School of Science(shenzhen), Harbin Institute of
Technology, Harbin, 150001, China*

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Abbreviations:

PPO	Phthaloyl peroxides
MPO	Malonoyl peroxides
BCTC	Brønsted base Covalently Tethered Carbonyl hypohalites
BHT	Butylated Hydroxytoluene
equiv.	Equivalent
HOMO	Highest Occupied Molecular Orbital
HAA	Hydrogen Atom Abstraction
LED	Light-Emitting Diode
LUMO	Lowest Occupied Molecular Orbital
NCR	Nitrogen-Centered Radical
OCR	Oxygen-Centered Radical
SOMO	Singly Occupied Molecular Orbital
TBAB	Tetrabutylammonium bromide
TBABr₃	Tetrabutylammonium tribromide
TDRA	Tether-tunable Distonic Radical Anion
TEMPO	2,2,6,6-Tetramethylpiperidinoxy
TMA	Tetramethylammonium

1. General information

1.1 Materials and Methods

All reagents were purchased from Energy, Sigma-Aldrich, Tansoole, Alfa Aesar, or TCI, and used without further purification. The reaction solvent, 1,2-dichloroethane and acetonitrile, was used without purification. Reactions were monitored by thin layer chromatography (TLC) and visualized by UV lamp (254 nm) or by staining with a solution of phosphomolybdic acid in EtOH followed by heating. Flash column chromatography was performed using 230-400 mesh silica gel. Yields refer to purified compounds unless otherwise noted.

¹H NMR (400 MHz), ¹³C NMR (100 MHz) spectra were obtained on Q.One Instruments 400M nuclear resonance spectrometers. ¹H NMR and ¹³C NMR chemical shifts are referenced with respect to CDCl₃ (¹H NMR: residual CHCl₃ at δ 7.26, ¹³C NMR: CDCl₃ triplet at δ 77.16) and CD₃CN (¹H NMR: residual CH₃CN at δ 1.94, ¹³C NMR: CD₃CN heptet at δ 1.32). Data for ¹H NMR spectra were reported as chemical shifts (δ ppm), broad peak (b), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, h = hextet, m = multiplet), coupling constant (Hz) and integration; data for ¹³C NMR were reported in terms of chemical shift (δ ppm) and no special nomenclature is used for equivalent carbons.

HR-ESI-MS spectra were recorded on a Bruker Esquire LC mass spectrometer using electrospray ionization. UV-Vis spectra were recorded on an Shimadzu 2600 spectrophotometer. The electron paramagnetic resonance (EPR) experiments were performed with a Bruker Elexsys E500 X-band spectrometer.

The stability of phthaloyl peroxide have been examined, which is insensitive to direct heating, shock, crush and scrape. Thermogravimetric analysis (TGA) data has shown that phthaloyl peroxide is stable below 90 °C. Rapid loss of mass occurs at 110 °C, indicating an exothermic decomposition at that temperature. Differential scanning calorimetry (DSC) data for cyclopentyl malonoyl peroxide shows an onset temperature of 70 °C. However, all peroxides might be dangerous under inappropriate conditions. These test data have been presented in the *references*^{1,2}.

1.2 The Reaction setup:

a. A 25 mL reaction vials was placed at the center of a stir plate. Two parallel 40W LEDs lamps are placed perpendicular to the sidewall of reaction vials, so that the reactions vials can be equally exposed to the LEDs. A fan is always turned on during the reaction, which is necessary in order to offset the heat generated from the LEDs light for reproducible results.



Figure S1. Details for the ring-opening halogenation reaction setup

b. A 25 mL reaction vials was placed at the center of a stir plate under the natural light or blue LEDs.

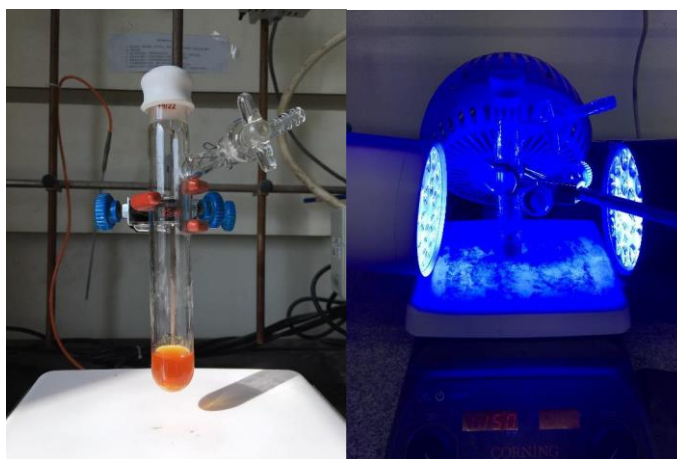


Figure S2. Details for the C(sp³)-H amination reaction setup

2. Detailed description of tethering PCET strategies

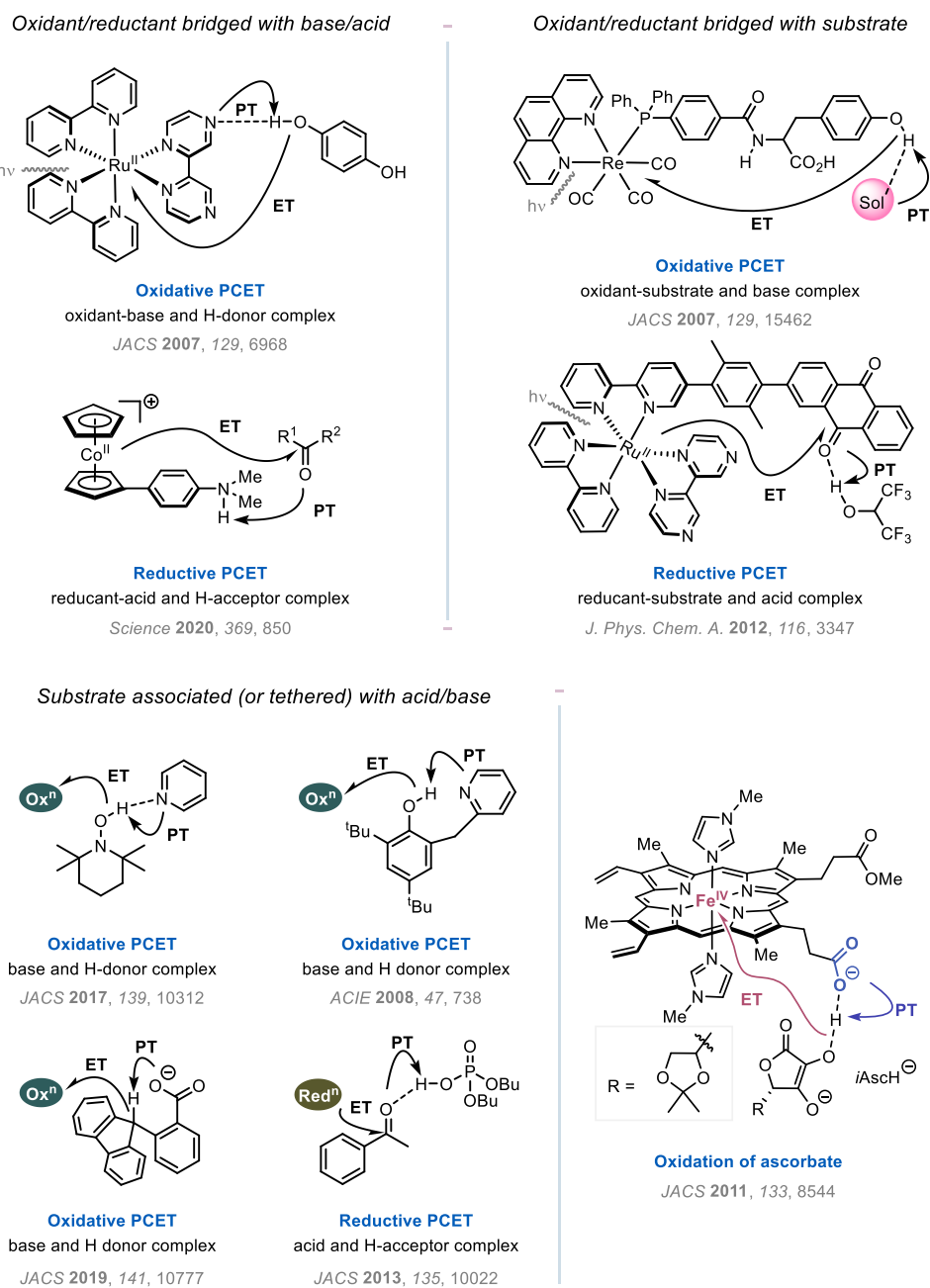


Figure S3. Some selected tethering PCET strategies³⁻¹¹

Benefiting from the research approach of proximity effects in enzyme chemistry, tethering strategies have long emerged in the field of organic chemists, with silicon-containing linkage structures being the earliest studied tethering structures.

In the early stages of the development of tethering strategies, the definition of tethering strategies was relatively narrow and involved the use of assembled and detachable bridging/tethering groups to connect two reaction sites and temporarily form a whole. After the reaction is complete, the binding groups need to be removed. This definition emphasizes that the formed single-molecule precursor can be separated or

identified, and the overall steps are mainly divided into three steps: preassembly, reaction, and removal of tethered groups, while the reaction of in situ preassembly to form intermediates is not included.

With the further development of tethering strategies, "tethering" has been recognized and used by more researchers as a way of thinking, and tethering strategies are no longer limited to early definitions. Adding binding groups to a wide variety of catalysts, reagents, and substrates provides researchers with a new perspective on reactivity. Therefore, after systematically summarizing the literature with tethering ideas reported thus far, tethering strategies can be divided into the following three categories based on the effects of tethering: 1) regulating the distance between reaction sites. This type of tethering strategy mainly targets reactants, converting intermolecular reactions into intramolecular reactions. This traditional tethering strategy can be divided into three main steps: preassembly, reaction, and removal. 2) Increased conformational limitations. This type of tying strategy mainly targets catalysts and reagents, and the addition of tying groups will help improve the selectivity of the reaction. 3) Addition of new activation groups. This type of tethering strategy can target both catalysts and reactants, and the added activation groups can provide new targets for the reaction.

3. Detailed description of Heteroatom-Centered radicals

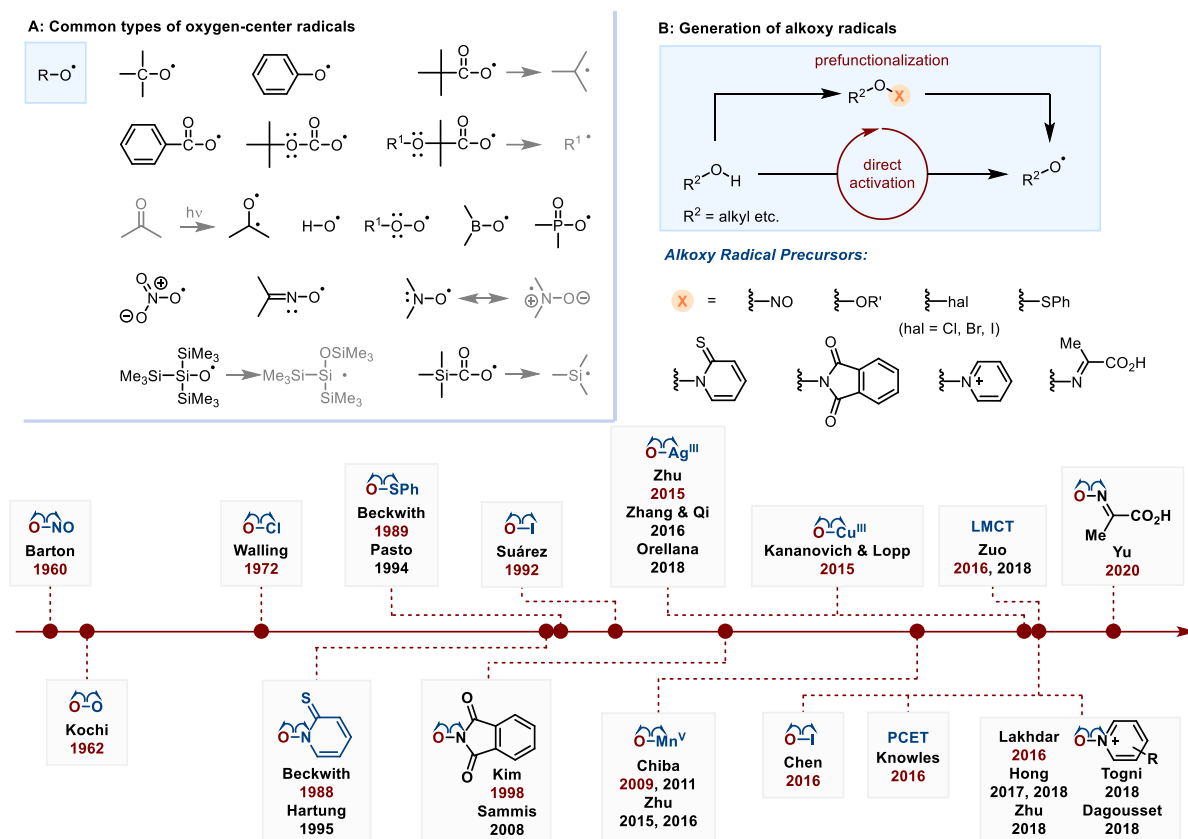


Figure S4. Methods for alkoxy radical generation

Alkoxy radicals are mainly generated by the cleavage of O–H bonds. Due to the high bond dissociation energy of O–H bonds in alcohols (O–H BDE \approx 105 kJ/mol), and the presence of C–H bonds with lower dissociation energy in molecules, direct homolytic activation of O–H bonds is very difficult. To overcome this difficulty, early chemical researchers indirectly achieved the breaking of oxygen hydrogen bonds by converting oxygen hydrogen bonds into weak oxygen heteroatom bonds, and developed a series of pre activated functional groups based on nitrogen atoms, sulfur atoms, and iodine atoms, including nitrite, peroxides, hypochlorous acids^{12–17}. Since 2000, research on the generation of alkoxy radicals has mainly focused on transition metal mediated single electron oxidation pathways, Proton coupled electron transfer (PCET), Ligand to metal charge transfer (LMCT), and mild and uniquely reactive pre activated functional groups^{18–24}

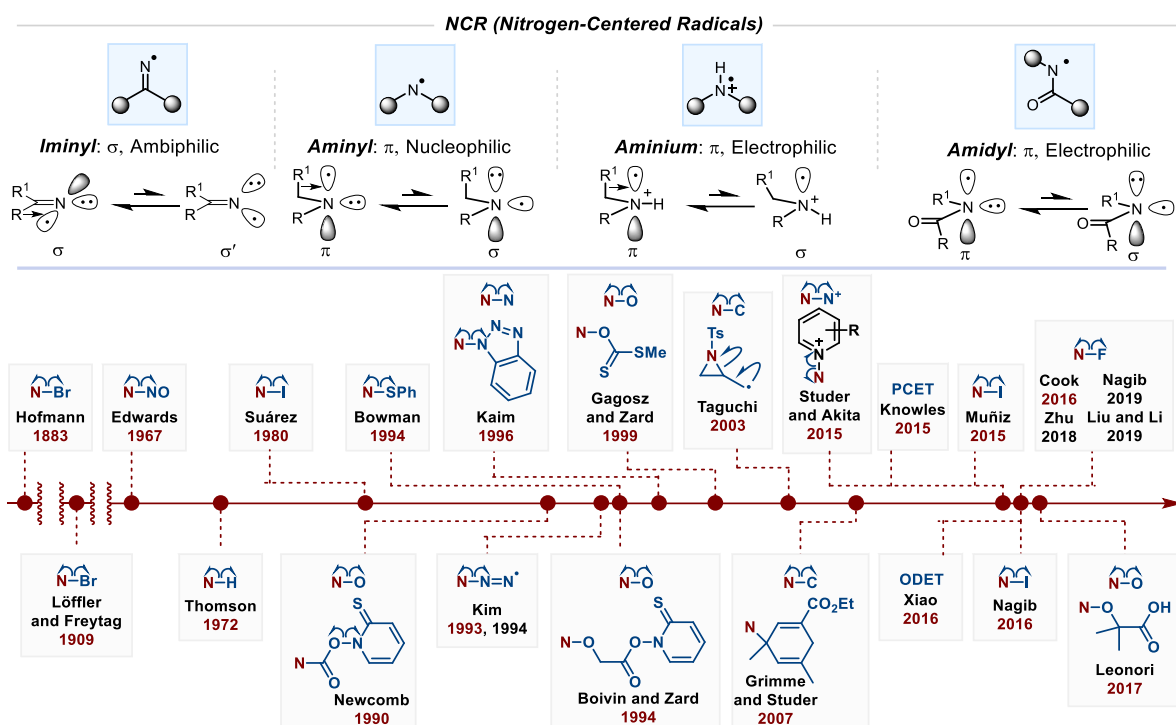


Figure S5. Methods for nitrogen centered radical generation

The earliest reported reaction for generating nitrogen atom center radicals through organic synthesis was the Hoffman Löffler Freytag (HLF) reaction. In 1883, Hofmann accidentally discovered that linear amines reflux in sulfuric acid in the presence of N-bromopyridine, producing pyrrolidine products²⁵. 26 years later, Löffler and Freytag synthesized nicotine using a similar pathway, confirming this unexpected discovery²⁶.

To maintain the high activity of nitrogen center radicals while avoiding acidic conditions, the Suárez research group connected electron withdrawing groups (such as NO₂, Boc) to nitrogen atoms, increasing the BDE value of N–H bonds, making it easier for the generated nitrogen radicals to complete the subsequent 1,5-hydrogen migration process. The mild conditions of adding oxidants to the iodine element used by the Suárez research group can also avoid using chlorine or bromine atoms as leaving groups, and use iodine atoms as leaving groups to achieve weak N–I bond cleavage²⁷. In 2015, the Muñiz research group improved the method by reducing the amount of iodine to the catalytic level, achieving the transformation from N–Ts amide to pyrrolidine product. However, this methodology still relies on the easily broken benzyl C–H bond substrate²⁸. In 2016, the Nagib research group reported on the HLF reaction using I₃[−] as a key active intermediate²⁹. By combining NaI with PhI(OAc)₂, inorganic iodized salts will slowly generate iodine monomers in situ, reducing the generation of highly active AcOI intermediates. The iodine elemental stored in I₃[−] will reduce the generation of by-products, making it possible for the HLF reaction of non-activated C–H bond substrates.

In addition to N–halogen bond cleavage, N–N bond cleavage³⁰, N–O bond cleavage^{31–33}, N–C bond cleavage^{34,35}, and N–F bond cleavage^{36–39}, are also effective methods for generating nitrogen center radicals.

4. Experiments data of excluding *in situ* formation of O–halogenated or N–halogenated intermediate

4.1 NMR evidence of excluding *in situ* formation of O–halogenated intermediate

NMR evidence for excluding the formation of hypobromite intermediate.

As described in Figure 2 in the manuscript, the alkoxy radical in the ring-opening halogenation of cycloalkanols could be generated by either the homolysis of O–Br bond of hypobromite or the direct homolysis of O–H bond of the corresponding cycloalkanol. From this point of view, we operated the reaction system under the optimization condition in the absence of light to avoid the possible PCET pathway, in order to verify whether the *in situ* formation of O–halogenated intermediate pathway represents the major pathway of this reaction. A series of NMR studies are presented as follows:

4.1.1. ¹³C NMR characterization of three typical hypobromites:

Initially, we synthesized the corresponding hypobromites of 1-phenylcyclohexanol, 1-methylcyclohexanol and 1-phenylcyclobutanol by employing the methodology reported by Matheny et al⁴⁰ in 1964. For the sake of clarity, the impurity substance in pentane (purchased from Energy, 99.5%), hypobromites, byproducts of reaction system, ring-opening halogenation product were labeled in purple, red, green and yellow, respectively.

The conversion of substituted six-membered cycloalkanols could finish in 30 minutes, the NMR of which demonstrated that the corresponding hypobromites were obtained as main product (**Figure S6, b and c**). For convenient comparison, the strong carbon resonates at 36.0-36.5 (C) were employed as the signal of the existence of hypobromites in PPO induced ring-opening halogenation.

For four-membered cycloalkanols, on the other hand, we failed to observe the directly generation of the corresponding hypobromites under the same reaction condition. Based on the reported NMR data, it was convincing that the ring-open bromination product was obtained instead of four-membered hypobromite, plausibly due to the relatively weak O–Br bond which caused by the stabilization of alkoxy radical by donation from strained ring. Alternatively, similar substrate had been subjected to a series of reaction conditions (including Br₂/AgSO₄, Br₂/NaOH, Br₂/HgO) by Singleton et al⁴¹. expecting to form the corresponding hypobromite, however, the ring-open bromination product was also formed as the major product.

Additionally, discernible carbon resonates (12.2, 13.4, 21.5, 32.4, 43.9) belong to the byproducts in reaction system of pentane, Br₂ and HgO.

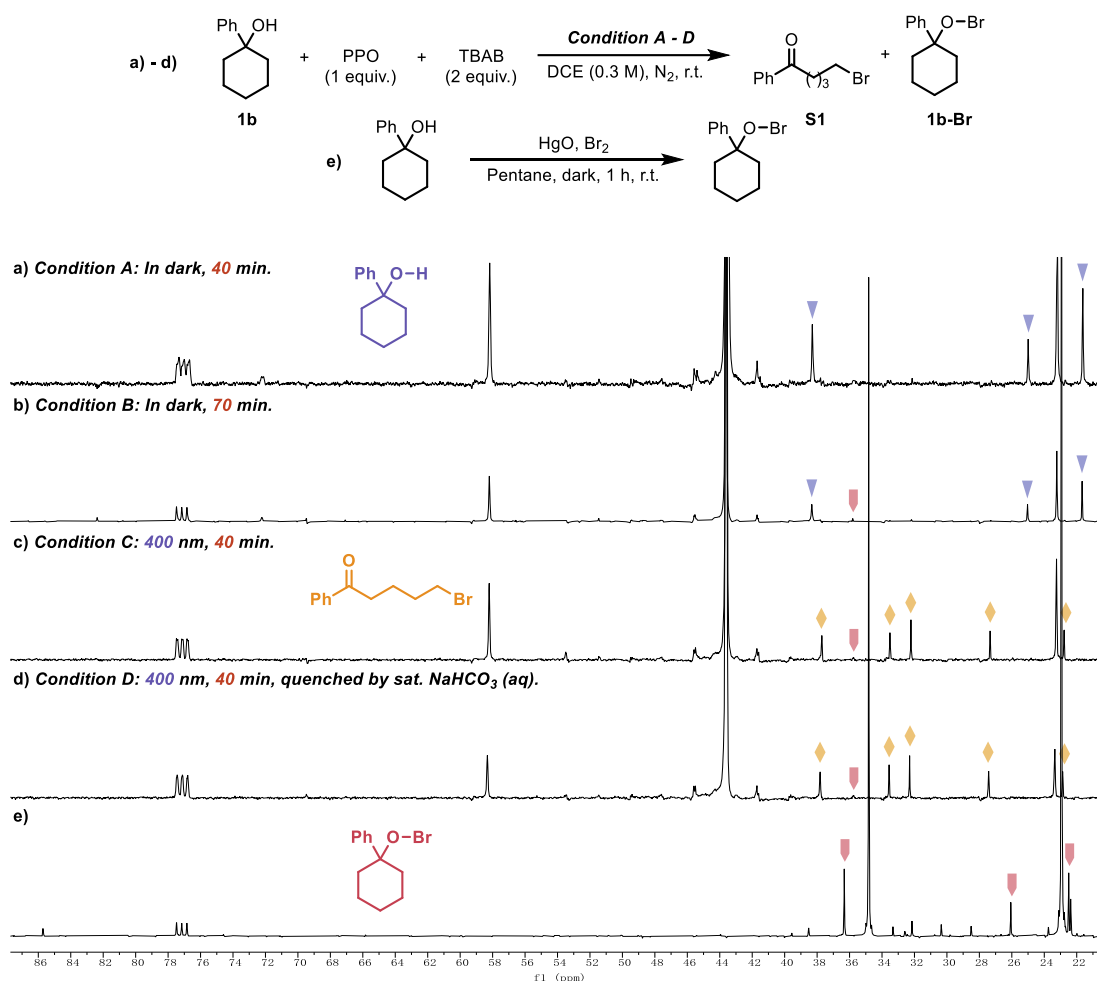


Figure S7. ¹³C NMR of PPO-induced ring-opening bromination of 1-phenylcyclohexan-1-ol **1b-Br** under different reaction conditions

The additional example shown below substantiate the same viewpoint of the low contribution of the polarity pathway to the PPO-induced ring-opening bromination of cycloalkanols. While phenyl was replaced by methyl, the corresponding bromination linear ketones **S2** could be obtained in 86% yield in 40 minutes under the irradiation of visible light (**Figure S8**) with the starting material completely consumed (**Figure S8, a and c**). low conversion of starting material was observed while operating the reaction in the absence of light, the result of which was in line with our viewpoint (**Figure S10, b and c**). Mechanically, due to the intrinsic strained ring difference of four- and six-membered cycloalkanols, the mechanism of the ring-opening bromination of two kinds of compounds was also different (concerted mechanism and stepwise mechanism). Therefore, we also tested the contribution of polarity pathway for the PPO-induced ring-opening of four-membered cycloalkanols. As shown in **Figure S11**, although the hypobromite intermediate **1a-Br** proceeded a rapid ring-opening reaction to afford the corresponding ring-opening product **2**, a low yield was detected (16%).

In conclusion, we verified that the polarity pathway is incapable of the visible-light-enhanced PPO-induced ring-opening halogenation of cycloalkanols on the basis of a series of NMR studies on different reaction system. In other words, the PECT-induced radical pathway promoted by covalently tethered distonic radical anion represents the major pathway of this efficient transformation

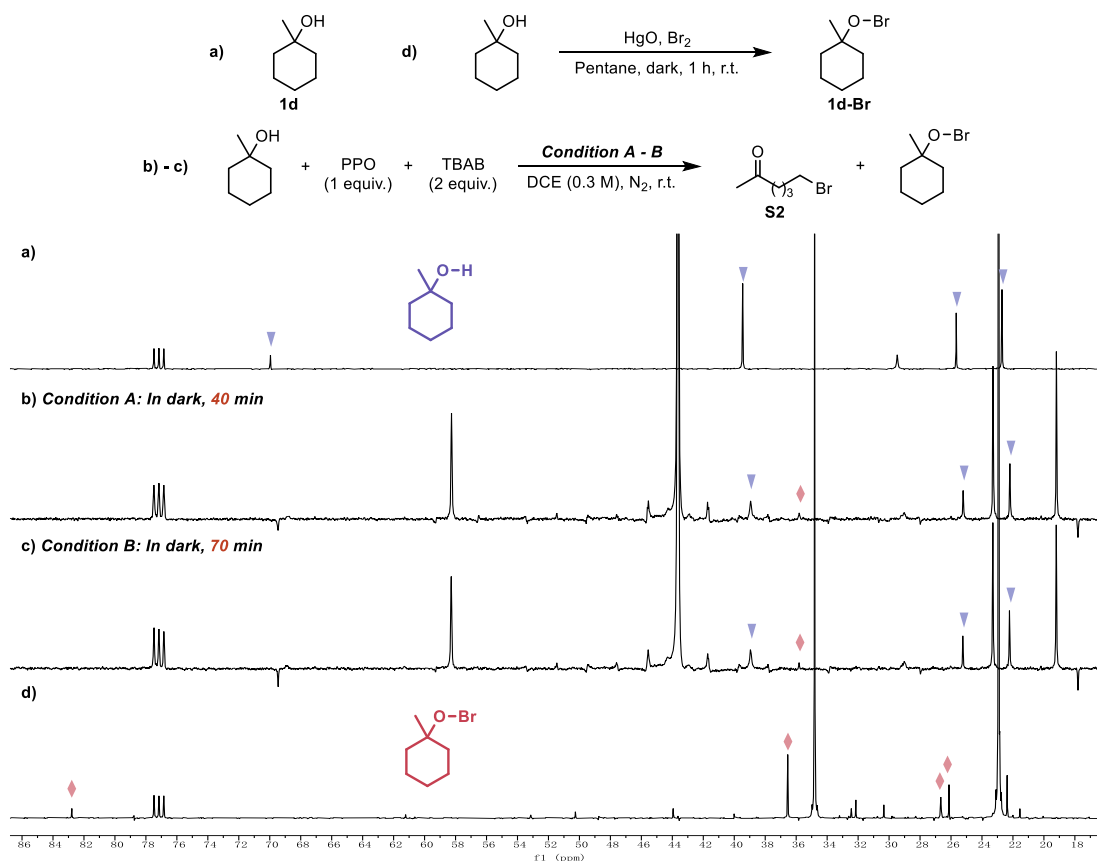


Figure S10. ^{13}C NMR of PPO-induced ring-opening bromination of 1-methylcyclohexan-1-ol **1d** in dark

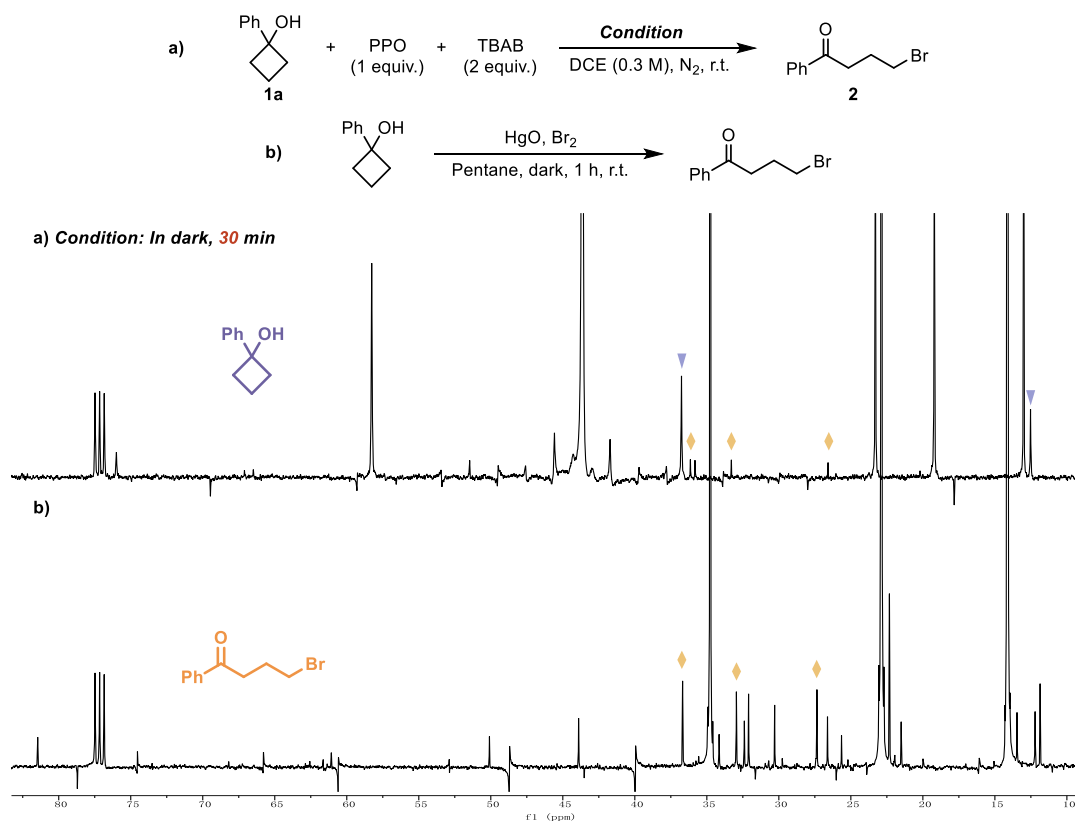


Figure S11. ^{13}C NMR of visible-light-promoted PPO-induced ring-opening bromination of 1-phenylcyclobutan-1-ol **1a** in dark

4.2 NMR evidence of excluding *in situ* formation of N-halogenated intermediate

4.2.1. NMR evidence of reaction mixture under dark condition

General Procedure: CsI (0.225 mmol, 3.0 equiv) was added to the NMR tube wrapped with the tinfoil. Acetonitrile-D₃ (0.75 mL) and imidate (0.075 mmol, 1.0 equiv) were added subsequently. MPO (0.225 mmol, 3.0 equiv) was added to the NMR tube under the dark condition. The mixture was bubbled with N₂ for 15 min under the dark condition. The tinfoil-wrapped NMR tube was then shaken for 2 h.

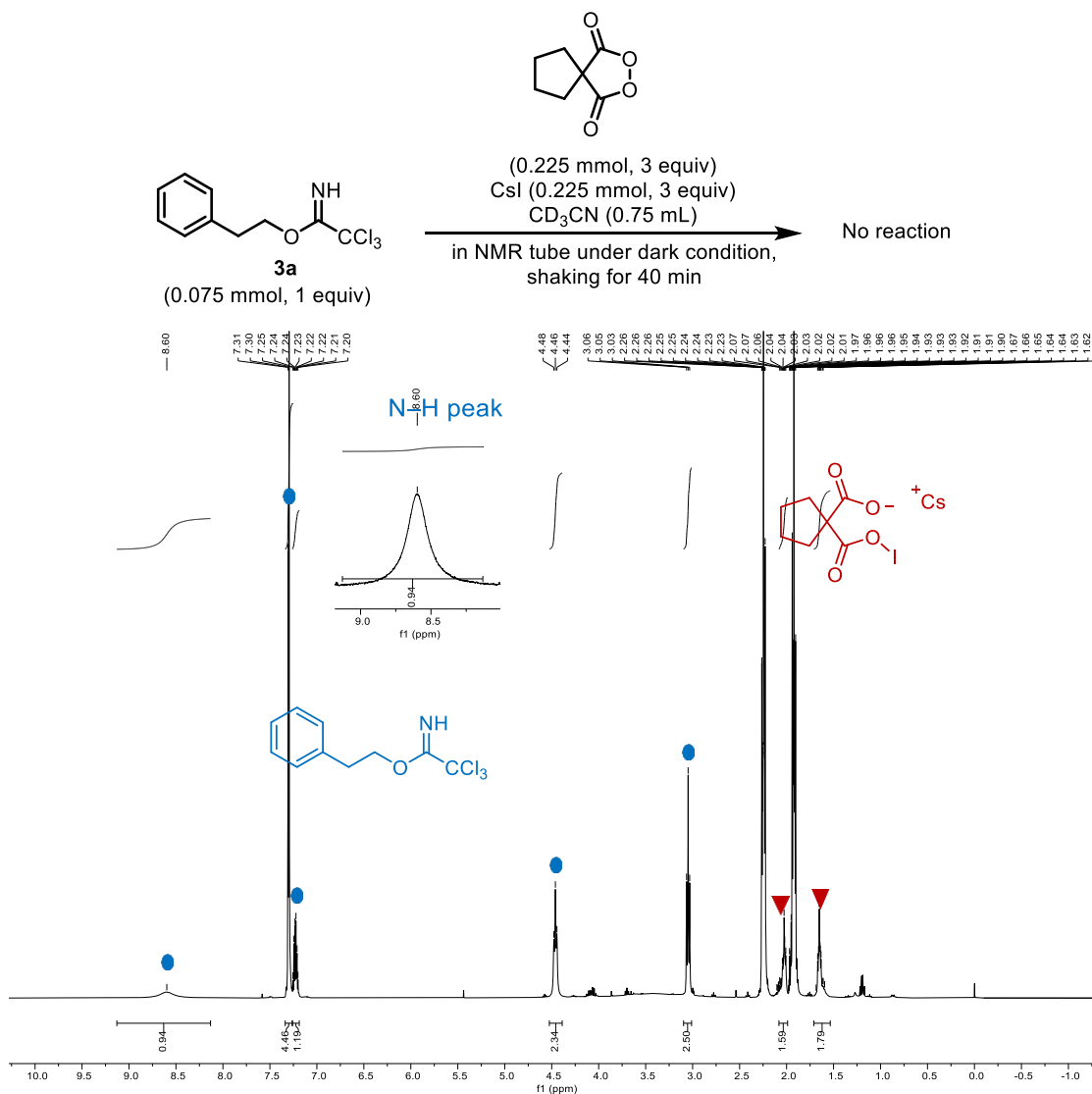


Figure S12. The ¹H NMR of the reaction mixture of **3a** in dark condition

General Procedure: CsI (0.225 mmol, 3.0 equiv) was added to the NMR tube wrapped with the tinfoil. Acetonitrile-D₃ (0.75 mL) and imidate (0.075 mmol, 1.0 equiv) were added subsequently. MPO (0.225 mmol, 3.0 equiv) was added to the NMR tube under the dark condition. The mixture was bubbled with N₂ for 15 min under the dark condition. The tinfoil-wrapped NMR tube was then shaken for 2 h.

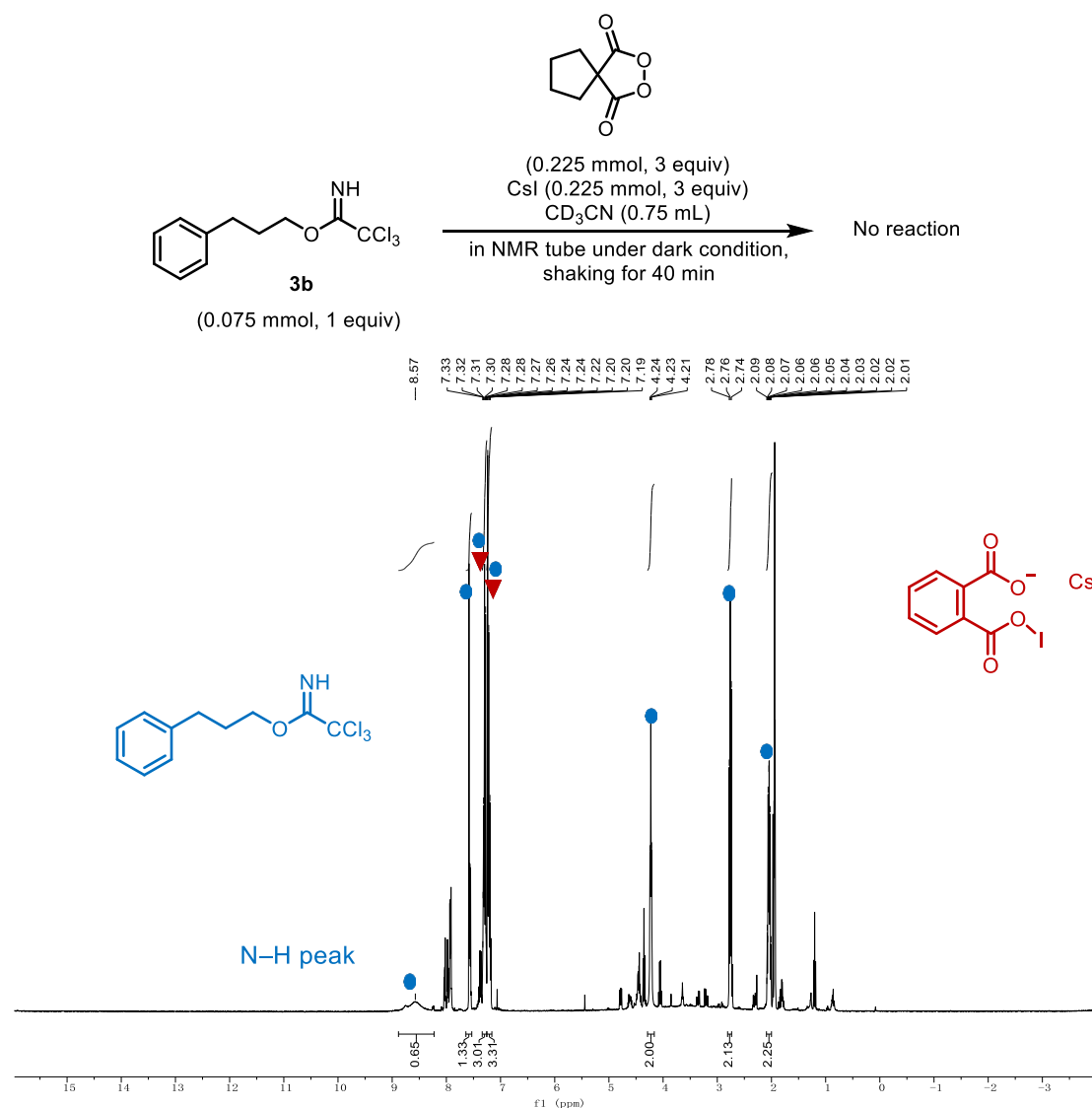


Figure 13. The ^1H NMR of the reaction mixture of **3b** in dark condition

After the *in situ* NMR experiments in dark condition, no product was observed in the ^1H NMR (**Figure S12** and **S13**). Especially, the existence of the N–H peak in ^1H NMR indicated that the cleavage of N–H bonds, even the likely halogenation of N–H bonds, did not occur under dark condition. Therefore, no reaction of imidates takes place during the degassed procedure.

We noticed that there may be nearly no difference between the NMR peaks of acyl hypiodite ($\text{R}-\text{CO}_2\text{I}$) and the NMR peaks of MPO and PPO. So, we performed the NMR experiment to *in situ* generate acyl hypiodite ($\text{R}-\text{CO}_2\text{I}$), suggesting acyl hypiodite ($\text{R}-\text{CO}_2\text{I}$) is generated (**Section 5.1**). The NMR spectra (**Section 5.1**) indicated that there is acyl hypiodite ($\text{R}-\text{CO}_2\text{I}$) in **Figure S12** and **S13**.

4.2.2. N–I derivatives

The stabilities of the N-halogenated compounds display drastically different behavior. As depicted in **Figure S13**, the relative stability of the halogenated tosylamides decreases in the order $\text{I} > \text{Br} > \text{Cl} > \text{F}$, while the reactivity increases by the inverse. We failed to isolate **3a-I**, but successfully isolated derivative **3a-Br** (**Figure S14**). Therefore, **3a-I** can not be used as a NMR reference pure compound.

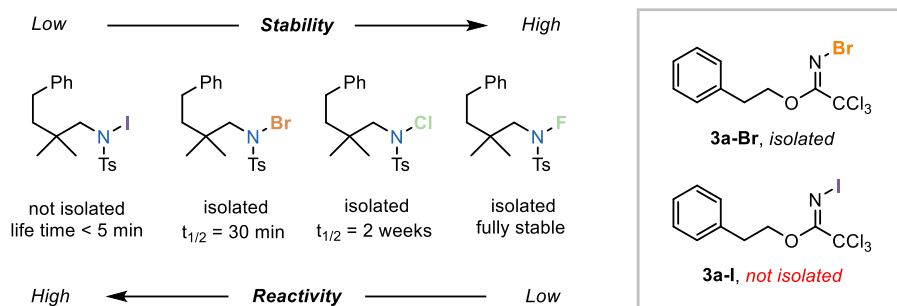
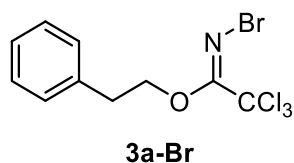


Figure S14. The stability and reactivity of N-halogenated compounds⁴³

4.2.3. Preparation of the N-Br intermediate

Two different stock vials were prepared: The first vial was added imidate (0.1 mmol) and MeCN (0.7 mL). N-Bromosuccinimide (0.2 mmol) and (Diacetoxyiodo)benzene (0.2 mmol) were added into the second vial. The contents of both vials were added into an NMR tube and once the combined solutions were mixed, the measurement was performed immediately.



pale yellow oil; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.35-7.28 (m, 2H), 7.27-7.19 (m, 3H), 4.54 (t, $J = 7.0$ Hz, 2H), 3.06 (t, $J = 6.9$ Hz, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 162.0, 136.6, 129.1, 128.8, 127.1, 89.9, 69.8, 34.8; **GC-MS (EI)**: m/z (%): 343, 117, 104 (100), 91, 77, 65, 51; **HRMS (ES⁺)** exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{10}\text{H}_9\text{BrCl}_3\text{NO}$) requires m/z 343.9006, found m/z 343.9022.

4.2.4. Preparation of the N-I intermediate

Two different stock vials were prepared: The first vial was added imidate (0.1 mmol) and MeCN (1 mL). I_2 (0.2 mmol) and (Diacetoxyiodo)benzene (0.2 mmol) were added into the second vial. The contents of both vials were added into an NMR tube and once the combined solutions were mixed, the measurement was performed immediately.

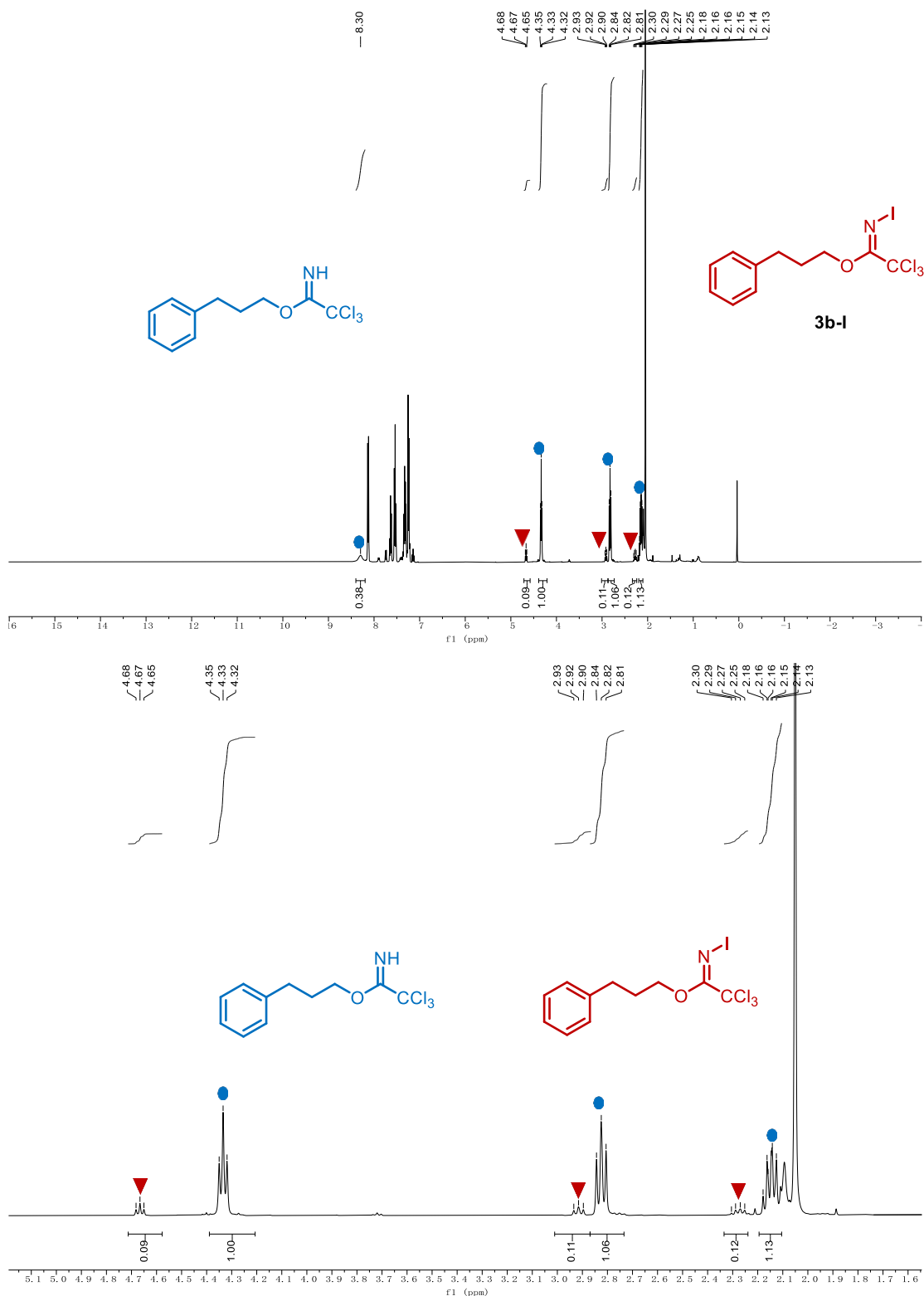


Figure S15. ^1H NMR spectrum used for the detection of N-I (top: full spectrum; bottom: zoom at the aliphatic part)

4.2.5. Detection of the reaction mixture

General Procedure: CsI (0.225 mmol, 3.0 equiv) was added to the NMR tube wrapped with the tinfoil. Acetonitrile- D_3 (0.75 mL) and imidate (0.075 mmol, 1.0 equiv) were added subsequently. MPO (0.225 mmol, 3.0 equiv) was added to the NMR tube. The mixture was stirred with N_2 for 30 min under the blue

LED. The tinfoil-wrapped NMR tube was then detected.

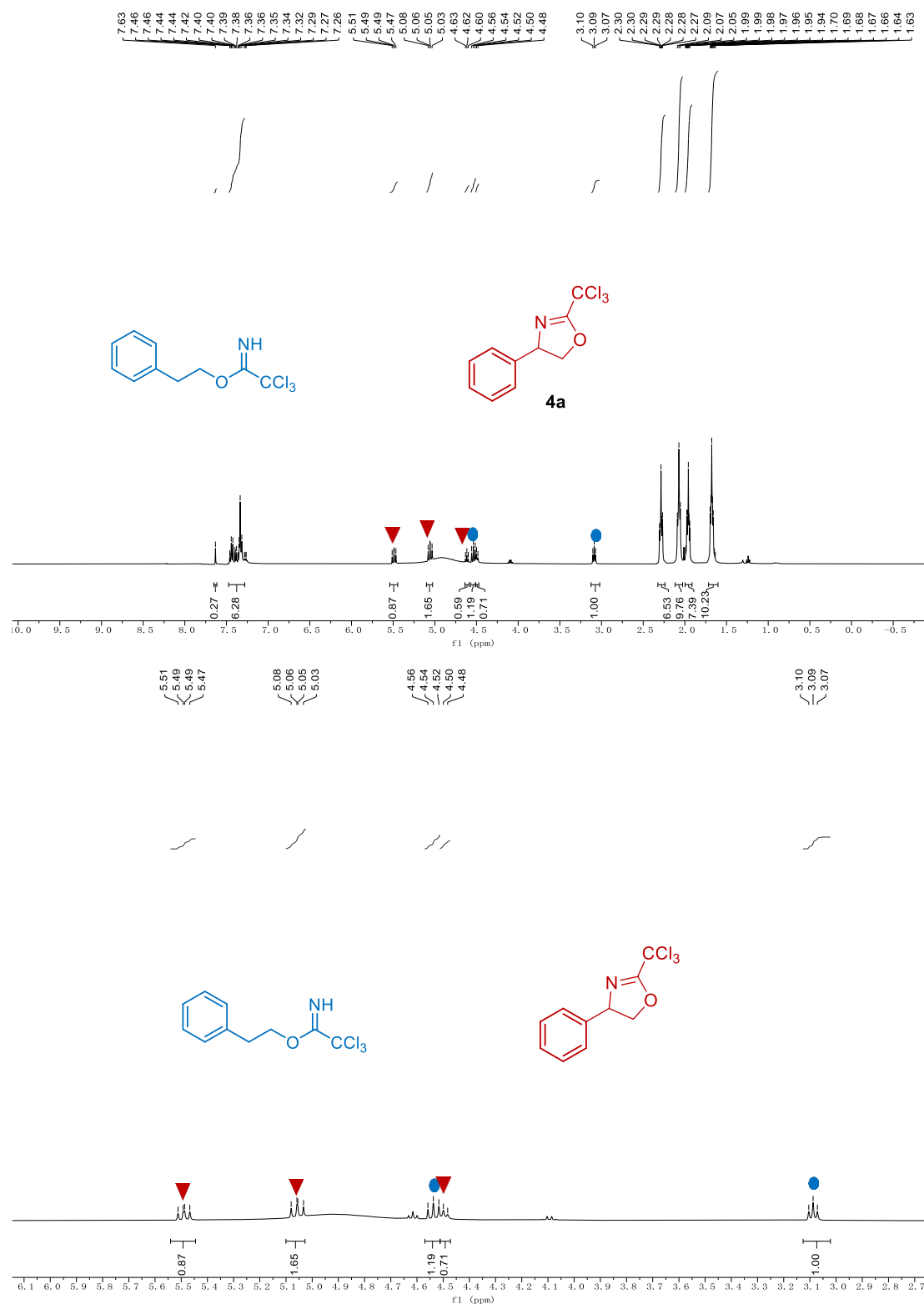


Figure S16. ^1H NMR spectrum used for the detection of reaction mixture (top: full spectrum; bottom: zoom at the aliphatic part)

General Procedure: CsI (0.225 mmol, 3.0 equiv) was added to the NMR tube wrapped with the tinfoil. Acetonitrile- D_3 (0.75 mL) and imidate (0.075 mmol, 1.0 equiv) were added subsequently. PPO (0.225 mmol, 3.0 equiv) was added to the NMR tube. The mixture was stirred with N_2 for 30 min under the blue LED. The

tin-foil-wrapped NMR tube was then detected.

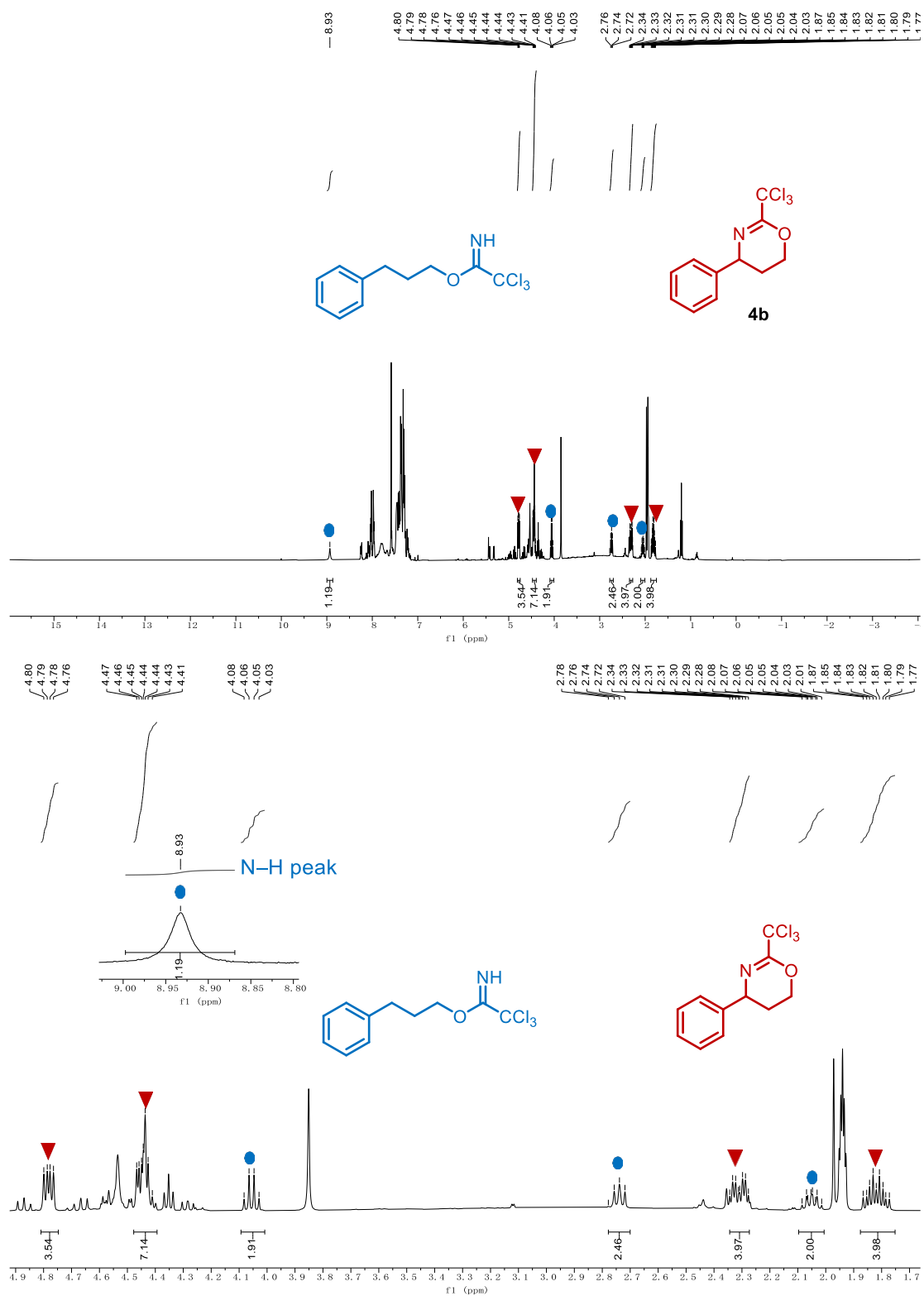
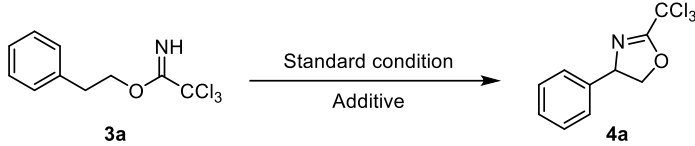


Figure S17. ¹H NMR spectrum used for the detection of reaction mixture (top: full spectrum; bottom: zoom at the aliphatic part)

4.3 Radical trap experiment

In order to further learn the mechanism of radical trapping, the β C(sp³)-H amination of imidate was operated with the addition of TEMPO and BHT as an additive in varying quantities or the reaction was run under typical conditions without degassing the reaction mixture. The isolated yields of oxazoline product and starting material are summarized in **Table S1**. Without any additive, oxazoline was isolated with 96% yield (**Table S1**, entry 1). The complete inhibition of β C-H amination was realized even with just 0.1 eq. TEMPO (**Table S1**, entries 2-4), which needs relatively larger quantities of BHT (**Table S1** entries 5-7).

Table S1 Quenching experiments of the β C-H amination of imidate

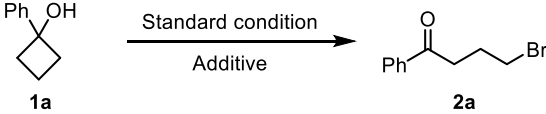


3a $\xrightarrow[\text{Additive}]{\text{Standard condition}}$ **4a**

Entry	Additive (equiv.)	Isolated yields of 4a	Recovery of 3a
1	/	96%	0%
2	TEMPO (0.1)	0%	93%
3	TEMPO (0.5)	0%	89%
4	TEMPO (1.0)	0%	92%
5	BHT (0.1)	45%	35%
6	BHT (0.5)	0%	84%
7	BHT (1.0)	0%	87%

A similar approach applies to the reaction of the ring-opening halogenation of cycloalkanols, TEMPO and BHT as an additive in varying quantities or the reaction was run under typical conditions without degassing the reaction mixture. The isolated yields of bromination linear ketones product and starting material are summarized in **Table S2**. Without any additive, bromination linear ketones was isolated with 96% yield (**Table S2**, entry 1). The complete inhibition of ring-opening halogenation was realized even with just 0.1 eq. TEMPO (**Table S2**, entries 2-4), which needs relatively larger quantities of BHT (**Table S2** entries 5-7).

Table S2 Quenching experiments of the ring-opening halogenation of cycloalkanols



1a $\xrightarrow[\text{Additive}]{\text{Standard condition}}$ **2a**

Entry	Additive (equiv.)	Isolated yields of 2a	Recovery of 1a
1	/	95%	0%
2	TEMPO (0.1)	0%	90%
3	TEMPO (0.5)	0%	91%
4	TEMPO (1.0)	0%	90%
5	BHT (0.1)	68%	22%
6	BHT (0.5)	0%	77%
7	BHT (1.0)	0%	90%

The difference between the results of TEMPO (entries 2-4) and BHT (entries 5-7) suggests that there are two different radical-trapping mechanisms of these two additives. The result in entry 2 implies that there is the radical-trapping catalytic cycle of TEMPO. Therefore, the carboxylic acids as the byproduct in our condition are one of the possible reasons to the highly efficient inhibition of TEMPO. In comparison, the stoichiometric factor for peroxy radical capture, for BHT is 2.0 in previous research, which means each BHT capture two peroxy radicals. Analogously, the stoichiometric factor of BHT is probably also smaller than that of TEMPO in our condition, which causes different radical-trapping results of TEMPO and BHT⁴⁴.

The radical adducts in the radical trap experiments were firstly probed. For reaction of C(sp³)-H amination of imidates, when BHT was used as the radical inhibitor, the radical adduct was successfully isolated (Table S3, entry 3,4); while no byproduct with TEMPO as the radical inhibitor was confirmed (Table S3, entry 1,2). Obviously, the reaction process was significantly suppressed by radical trap, as 2,2,6,6-tetramethylpiperidin-1-yloxy (TEMPO) and 2,6-di-*tert*-butyl-4-methylphenol (BHT).

General procedure for the radical trap experiments of C(sp³)-H amination: CsI (0.9 mmol, 3.0 equiv) was added to a 25 mL pressure tube under high vacuum with heating, and backfilled with N₂ (3 times). Dry acetonitrile (3 mL), imidate **3a** (0.3 mmol, 1.0 equiv), and additive (0.9 mmol, 3.0 equiv), were added under nitrogen atmosphere subsequently. MPO (0.9 mmol, 3.0 equiv) was added to the pressure tube in the end. The reaction was degassed using a freeze-pump-thaw technique (3 times), then added to the vial under N₂. The mixture was then stirred under sunlight until the starting material had been consumed as determined by TLC. After the reaction was finished, the mixture was quenched by 20% Na₂S₂O₃ (15 mL) and washed with CH₂Cl₂ (3 × 25 mL). The combined organic layers were dried over Na₂SO₄ and concentrated. The crude product was obtained 21% yield purified by flash chromatography on silica gel (PE/EA, 1% AcOH).

Table S3 The radical trap experiment and corresponding byproduct.

Entry	Substrate	Additive	Yields of 4a	Byproduct	Yields of Byproduct
1	3a	+ 3 equiv 	0%	Fail to confirm any byproduct with TEMPO	/
2	w/o 3a				/
3	3a	+ 3 equiv 	0%		16%
4	w/o 3a				21%

A similar approach applies to the reaction of the ring-opening halogenation of cycloalkanols, when BHT was used as the radical inhibitor, the radical adduct was successfully isolated (Table S4, entry 3,4);

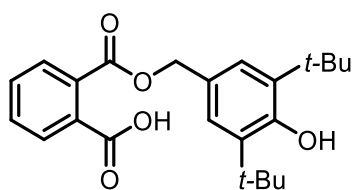
while no byproduct with TEMPO as the radical inhibitor was confirmed (**Table S4**, entry 1,2).

General procedure for the radical trap experiments of ring-opening halogenation: TBAB (0.3 mmol, 1.0 equiv) was added to a 25 mL pressure tube under high vacuum with heating, and backfilled with N₂ (3 times). Dry DCE (1 mL), **1a** (0.3 mmol, 1.0 equiv), and additive (0.9 mmol, 3.0 equiv), were added under nitrogen atmosphere subsequently. PPO (0.3 mmol, 1.0 equiv) was added to the pressure tube in the end. The reaction was degassed using a freeze-pump-thaw technique (3 times), then added to the vial under N₂. The mixture was then stirred under sunlight until the starting material had been consumed as determined by TLC. After the reaction was finished, the mixture was poured over 20% Na₂S₂O₃ (15 mL) and washed with CH₂Cl₂ (3 × 25 mL). The combined organic layers were dried over Na₂SO₄ and concentrated. The crude product was obtained 27% yield purified by flash chromatography on silica gel (PE/EA, 1% AcOH).

Table S4 The radical trap experiment and corresponding byproduct.

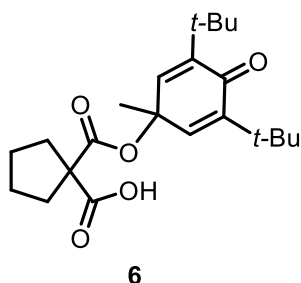
Entry	Substrate	Additive	Yields of 4a	Byproduct	Yields of Byproduct
1	1a	+ 3 equiv 	0%	Fail to confirm any byproduct with TEMPO	/
2	w/o 1a				/
3	1a	+ 3 equiv 	0%		18%
4	w/o 1a				27%

In summary, the radical inhibition experiments illustrate that there are radical intermediates including in our mechanism. Based on the BHT radical adduct, we proposed MPO and CsI or PPO and TBAB could form the radical intermediates before the incorporation of imidates and cycloalkanols, which is consistent with EPR experiments. The β C–H amination and the ring-opening halogenation of cycloalkanols was infinitely inhibited by TEMPO, which is speculated due to the carboxylic acid-promoted catalytic cycle. In addition, the BHT radical adduct also suggests the decarboxylation has low probability from another perspective.



5

¹H NMR (400 MHz, CDCl₃) δ 7.94 (dd, *J* = 7.2, 1.9 Hz, 1H), 7.71 (dd, *J* = 6.9, 1.9 Hz, 1H), 7.68 – 7.48 (m, 2H), 7.24 (s, 2H), 5.28 (s, 1H), 5.27 (s, 2H), 1.42 (s, 18H). **¹³C NMR** (101 MHz, CDCl₃) δ 171.22, 168.49, 154.30, 136.17, 133.53, 132.32, 131.03, 130.33, 130.11, 129.03, 126.26, 125.98, 69.03, 34.42, 30.31. **HRMS (ES⁺)** exact mass calculated for [M+H]⁺ (C₂₃H₂₉O₅) requires *m/z* 385.2010, found *m/z* 385.2014.

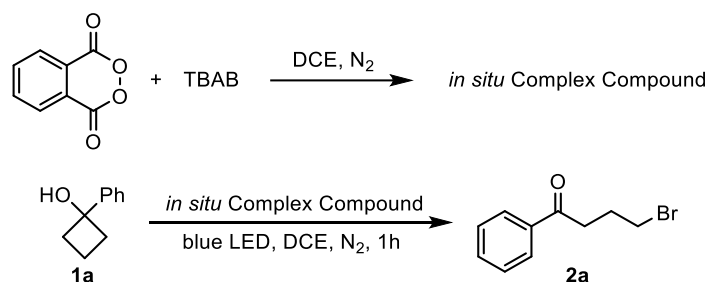


¹H NMR (400 MHz, CDCl₃): δ 6.53 (s, 2H; CH), 2.31-2.11 (m, 4H; CH₂), 1.77-1.66 (m, 4H; CH₂), 1.48 (s, 3H; CH₃), 1.22 (s, 18H; CH₃); **¹³C NMR** (100 MHz, CDCl₃): δ 186.4 (C=O), 177.6 (C=O), 170.7 (C=O), 146.5 (C), 139.9 (CH), 76.6 (C), 60.7 (C), 35.0 (CH₂), 34.8 (C), 29.5 (CH₃), 27.3 (CH₃), 25.7 (CH₂); **HRMS (ES⁺)** exact mass calculated for [M+Na]⁺ (C₂₂H₃₂O₅) requires *m/z* 399.2142, found *m/z* 399.2141.

4.4 Supplementary experiments

4.4.1 The effect of light on the ring-opening halogenation reaction

Table S5. The effect of light on the ring-opening halogenation reaction



Entry	Conditions	Time	Yield of 2a
1	blue LED 30 min	0.5 h	99%
2	no blue LED (under light condition)	0.5 h	22%
3	no blue LED (under light condition)	1 h	42%
4	no blue LED (under light condition)	12 h	63%
5	dark	0.5 h	18%
6	dark	1 h	22%
7	dark	12 h	60%

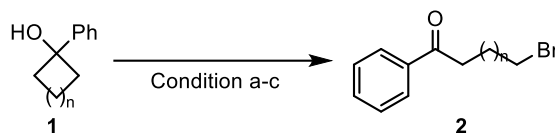
Experiments procedures:

In a reaction vial, TBAB (33 mg, 0.1 mmol, 1.0 equiv.) in dry DCE (0.5 mL) was added PPO (32 mg, 0.2 mmol, 2.0 equiv.) and substrate (0.1 mmol, 1.0 equiv.) was added. The mixture was stirred for different conditions. Under blue LED illumination, the desired product could be obtained in 99% yield in 30 minutes. Under natural light conditions, the yield was 22% in 30 minutes, 42% in one hour and 63% in 12 hours. Under dark conditions, the yield was 18% in 30 minutes, 22% in one hour and 60% in 12 hours.

4.4.2 The influence of different reaction conditions on the ring-opening halogenation reaction

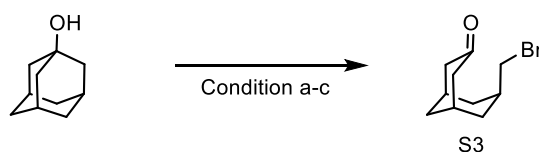
Table S6. The influence of different reaction conditions on the ring-opening halogenation reaction

Condition a: PPO(2.0 eq), TBAB(1.0 eq), DCE(0.3 M), r.t., blue LED
 Condition b: AgSO₄(1.2 eq), Br₂(1.0 eq), water(0.1 M), r.t.
 Condition c: K₂CO₃(6.0 eq), Br₂(5.0 eq), CHCl₃(0.3 M), 0 °C



Entry	Condition	n	Time	Yield
1	a	n=1	0.5 h	99%
2	b	n=1	0.5 h	53%(89%) ^a
3	c	n=1	0.5 h	59%(99%) ^a
4	a	n=5	2 h	38%
5	b	n=5	2 h	18%
6	c	n=5	2h	85%

^a stirred for 3h. ^b stirred for 5h.



Entry	Condition	Time	Yield
1	a	3 h	33%
2	b	3 h	23%
3	c	5 h	95%

Similar substrate had been subjected to a series of reaction conditions (including Br₂/AgSO₄, Br₂/NaOH, Br₂/HgO) by Singleton and Li et al. expecting expect to form the ring-open bromination product. Four-, eight-membered cyclic and Adamantane alcohols and were used to test the influences of different conditions. For reaction **condition b**, when the substrate is four-membered cyclic alcohols, the product can be obtained in 53% yield in half an hour and 99% yield in 3 hours; when the substrate is adamantane alcohols, the product can be obtained in 23% yield in half an hour. For reaction **condition c**, when the substrate is four-membered cyclic alcohols, the product can be obtained in 99% yield in 5 hours; when the substrate is eight-membered cyclic alcohols, the eight-product can be obtained in 85% yield; when the substrate is adamantane alcohols, the product can be obtained in 95% yield in 5 hours.

4.5 Experiment data of electron paramagnetic resonance

4.5.1 Set-up for the electron paramagnetic resonance studies

The electron paramagnetic resonance (EPR) experiments were performed with a Bruker Eleksys E500 X-band spectrometer. The spectral data was collected at 298 K with the following spectrometer settings: microwave power = 1.002 mW; sweep width = 100.0 G, modulation frequency = 100 kHz, sweep width amplitude = 0.0002 T, time constant = 0 ms, gain = 23 dB, conversion time = 0.0293 s, microwave frequency = 9.841332 GHz



Figure S18. Set-up for electron paramagnetic resonance (EPR) studies

4.5.2 Spin-trapping experiments with DMPO as trapping reagent

Sample (a): In a reaction vial, PPO (16 mg, 0.1 mmol, 1.0 equiv.) was dissolved in dry MeCN (0.5 mL), and DMPO (22 mg, 0.2 mmol, 2.0 equiv.) was added. The mixture was stirred for 10 minutes under blue LED. Then, the samples were filtered and transferred to quartz EPR tubes and the spectra were measured at 298 K.

Sample (b): In a reaction vial, TBAB (33 mg, 0.1 mmol, 1.0 equiv.) in dry MeCN (0.5 mL) was added PPO (16 mg, 0.1 mmol, 1.0 equiv.) and DMPO (22 mg, 0.2 mmol, 2.0 equiv.). The mixture was stirred for 10 minutes under blue LED. Then, the sample was filtered and transferred to quartz EPR tube and the spectrum was measured at 298 K.

Sample (c): In a reaction vial, TBAI (37 mg, 0.1 mmol, 1.0 equiv.) in dry MeCN (0.5 mL) was added PPO (16 mg, 0.1 mmol, 1.0 equiv.) and DMPO (22 mg, 0.2 mmol, 2.0 equiv.). The mixture was stirred for 10 minutes under blue LED. Then, the sample was filtered and transferred to quartz EPR tube and the spectrum was measured at 298 K.

Sample (d): In a reaction vial, CsI (26 mg, 0.1 mmol, 1.0 equiv.) in dry MeCN (0.5 mL) was added PPO (16 mg, 0.1 mmol, 1.0 equiv.) and DMPO (22 mg, 0.2 mmol, 2.0 equiv.). The mixture was stirred for 10 minutes under blue LED. Then, the sample was filtered and transferred to quartz EPR tube and the spectrum was measured at 298 K.

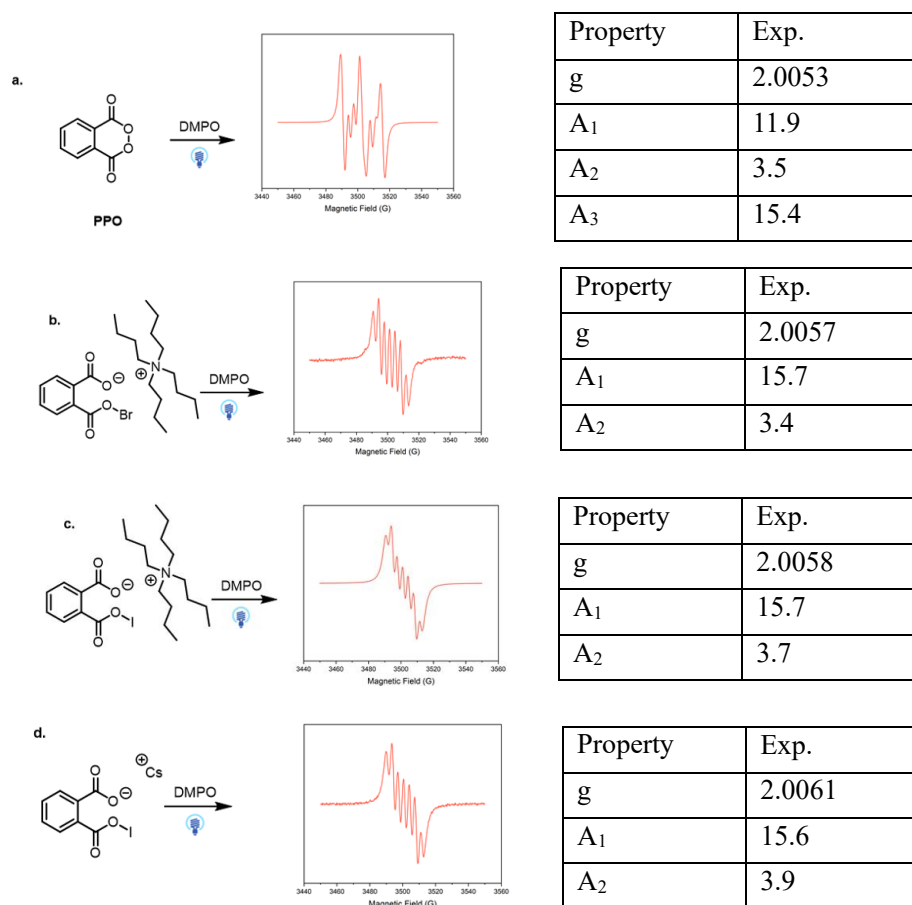
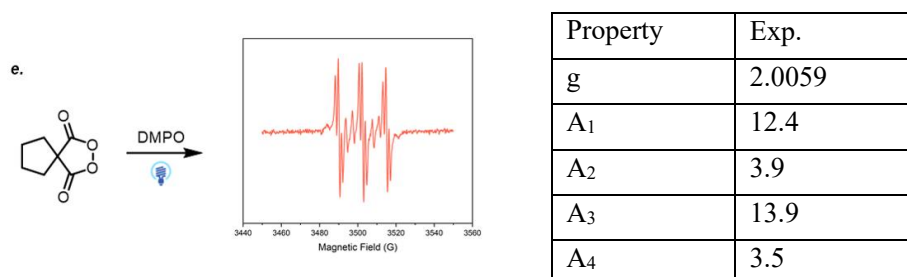


Figure S19. The EPR spectrum of PPO and DMPO(a); PPO with TBAB and DMPO(b); PPO with TBAI and DMPO(c); PPO with CsI and DMPO(d).

Sample (e): In a reaction vial, MPO (16 mg, 0.1 mmol, 1.0 equiv.) was dissolved in dry MeCN (0.5 mL), and DMPO (22 mg, 0.2 mmol, 2.0 equiv.) was added. The mixture was stirred for 10 minutes under blue LED. Then, the sample was filtered and transferred to quartz EPR tube and the spectrum was measured at 298 K.

Sample (f): In a reaction vial, TBAB (33 mg, 0.1 mmol, 1.0 equiv.) in dry MeCN (0.5 mL) was added MPO (16 mg, 0.1 mmol, 1.0 equiv.) and DMPO (22 mg, 0.2 mmol, 2.0 equiv.). The mixture was stirred for 10 minutes under blue LED. Then, the sample was filtered and transferred to quartz EPR tube and the spectrum was measured at 298 K.



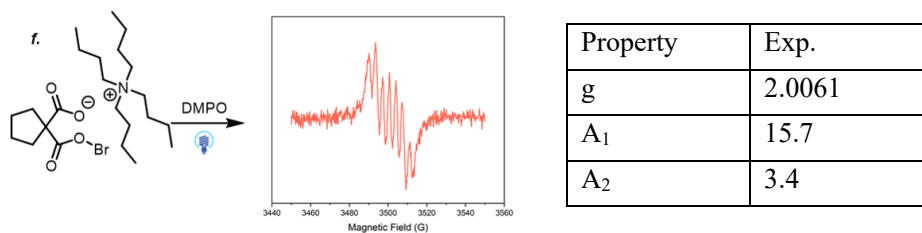


Figure S20. The EPR spectrum of MPO and DMPO(e); MPO with TBAB and DMPO(f).

Sample (g): In a reaction vial, CsI (26 mg, 0.1 mmol, 1.0 equiv.) in dry MeCN (0.5 mL) was added PPO (16 mg, 0.1 mmol, 1.0 equiv.) and DMPO (22 mg, 0.2 mmol, 2.0 equiv.). The mixture was stirred for 10 minutes, 30 minutes and 60 minutes under blue LED. Then, the samples were filtered and transferred to quartz EPR tubes and the spectra were measured at 298 K. The intensity of the signal in the EPR spectra was found time-dependent to the pronounced irradiation time

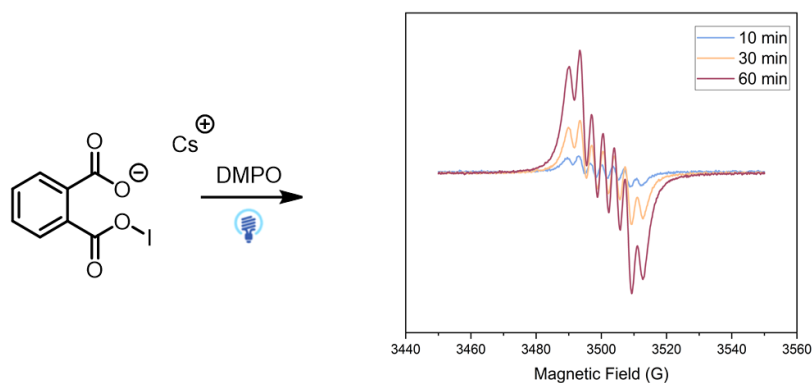


Figure S21. The EPR spectra of PPO with CsI and DMPO. Irradiation time: 10 min, 30 min, 60 min.

Sample (h): In a reaction vial, TBAB (33 mg, 0.1 mmol, 1.0 equiv.) in dry MeCN (0.5 mL) was added PPO (16 mg, 0.1 mmol, 1.0 equiv.) and DMPO (22 mg, 0.2 mmol, 2.0 equiv.). The mixture was stirred for 10 minutes, 30 minutes and 60 minutes under blue LED. Then, the samples were filtered and transferred to quartz EPR tubes and the spectra were measured at 298 K. The intensity of the signal in the EPR spectra was found time-dependent to the pronounced irradiation time.

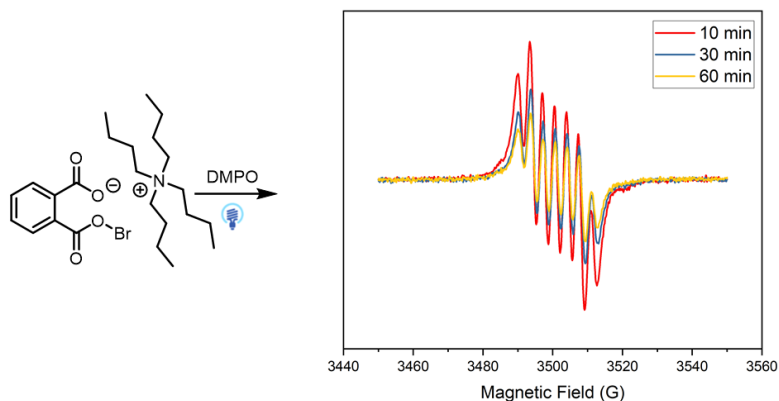


Figure S22. The EPR spectra of PPO with TBAB and DMPO. Irradiation time: 10 min, 30 min, 60 min.

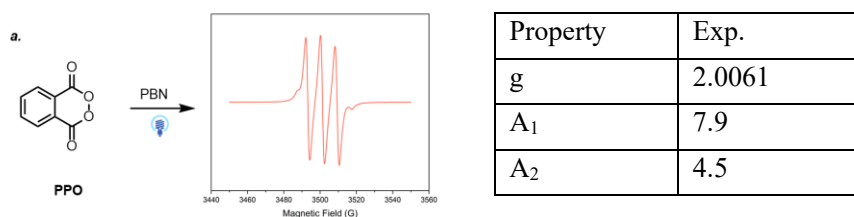
4.5.3 Spin-trapping experiments with PBN as trapping reagent

Sample (a): In a reaction vial, PPO (16 mg, 0.1 mmol, 1.0 equiv.) was dissolved in dry MeCN (0.5 mL), and PBN (35.4 mg, 0.2 mmol, 2.0 equiv.) was added. The mixture was stirred for 10 minutes under blue LED. Then, the samples were filtered and transferred to quartz EPR tubes and the spectra were measured at 298 K.

Sample (b): In a reaction vial, MPO (16 mg, 0.1 mmol, 1.0 equiv.) was dissolved in dry MeCN (0.5 mL), and PBN (35.4 mg, 0.2 mmol, 2.0 equiv.) was added. The mixture was stirred for 10 minutes under blue LED. Then, the sample was filtered and transferred to quartz EPR tube and the spectrum was measured at 298 K.

Sample (c): In a reaction vial, TBAB (32 mg, 0.1 mmol, 1.0 equiv.) in dry MeCN (0.5 mL) was added PPO (16 mg, 0.1 mmol, 1.0 equiv.) and PBN (35.4 mg, 0.2 mmol, 2.0 equiv.). The mixture was stirred for 10 minutes under blue LED. Then, the sample was filtered and transferred to quartz EPR tube and the spectrum was measured at 298 K.

Sample (d): In a reaction vial, CsI (26 mg, 0.1 mmol, 1.0 equiv.) in dry MeCN (0.5 mL) was added PPO (16 mg, 0.1 mmol, 1.0 equiv.) and PBN (35.4 mg, 0.2 mmol, 2.0 equiv.). The mixture was stirred for 10 minutes under blue LED. Then, the sample was filtered and transferred to quartz EPR tube and the spectrum was measured at 298 K.



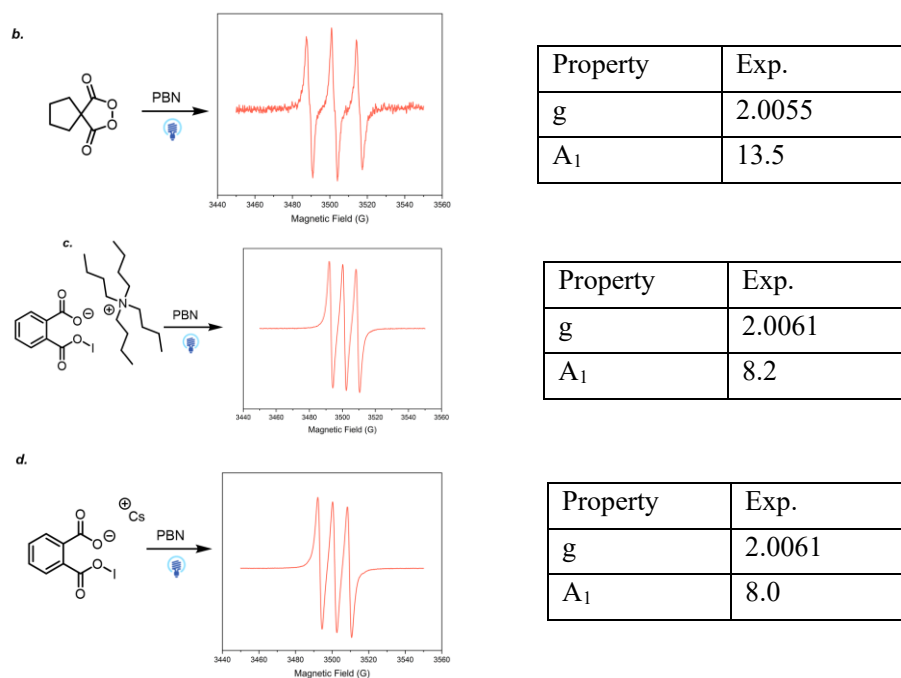


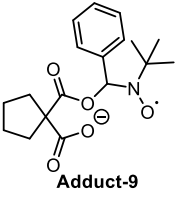
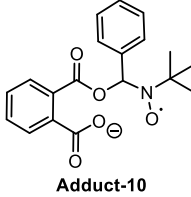
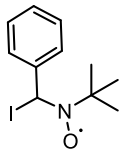
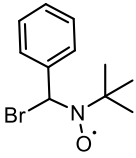
Figure S23. The EPR spectrum of **a.** PPO and PBN; **b.** MPO and PBN; **c.** PPO with TBAB and PBN; **d.** PPO with CsI and PBN.

Here we will demonstrate the predictive EPR properties and spectra using ORCA. The geometry can be optimized using B3LYP/Def2-TZVP and the g tensor and hyperfine coupling constants (HFCCs) for the atoms, using the B3LYP functional.

Table S7. Some predictive EPR properties using ORCA

Property (Sim.)	 Adduct-1	 Adduct-2	 Adduct-3	 Adduct-4
g	2.0057	2.0059	2.0062	2.0060
A	13.2, 2.6, 6.3	20.3, 10.3, 2.6, 2.2	19.6, 3.7, 2.6	11.2, 9.8, 1.8

Property (Sim.)	 Adduct-5	 Adduct-6	 Adduct-7	 Adduct-8
g	2.0059	2.0060	2.0063	2.0209
A	21.0, 2.7, 4.1, 2.0	16.0, 3.3, 5.4	16.2, 9.4, 4.2	11.4, 5.9, 2.9, 19.6, 129.2

Property (Sim.)	 Adduct-9	 Adduct-10	 Adduct-11	 Adduct-12
g	2.0061	2.0060	2.0063	2.0155
A	38.3	39.4	3.9, 4.0	24.5, 108.0

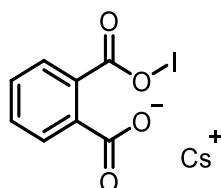
Because the EPR analysis on our spectra could not deduce the accurate structures of radical intermediates, we use these EPR results as the qualitative evidence of the radical mechanism enabled by cyclic diacyl peroxides.

5. Identification of Brønsted base Covalently Tethered Carbonyl hypohalites (BCTC)

5.1 NMR evidence of BCTC

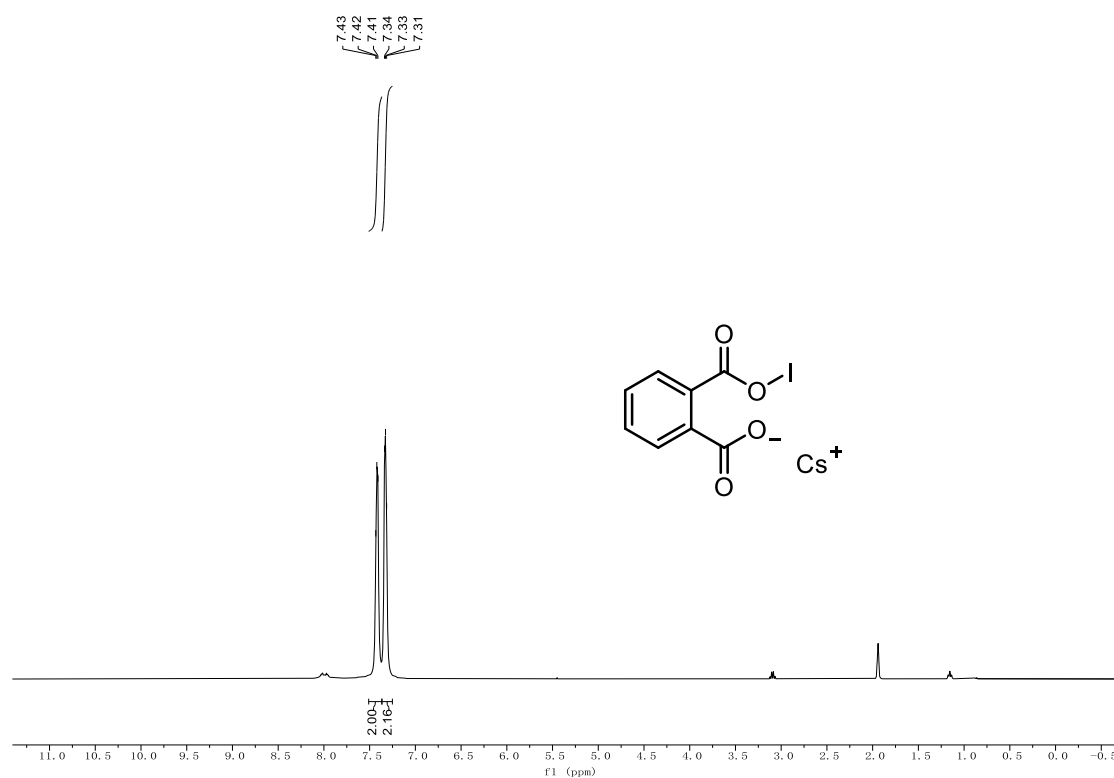
5.1.1 PPO + CsI

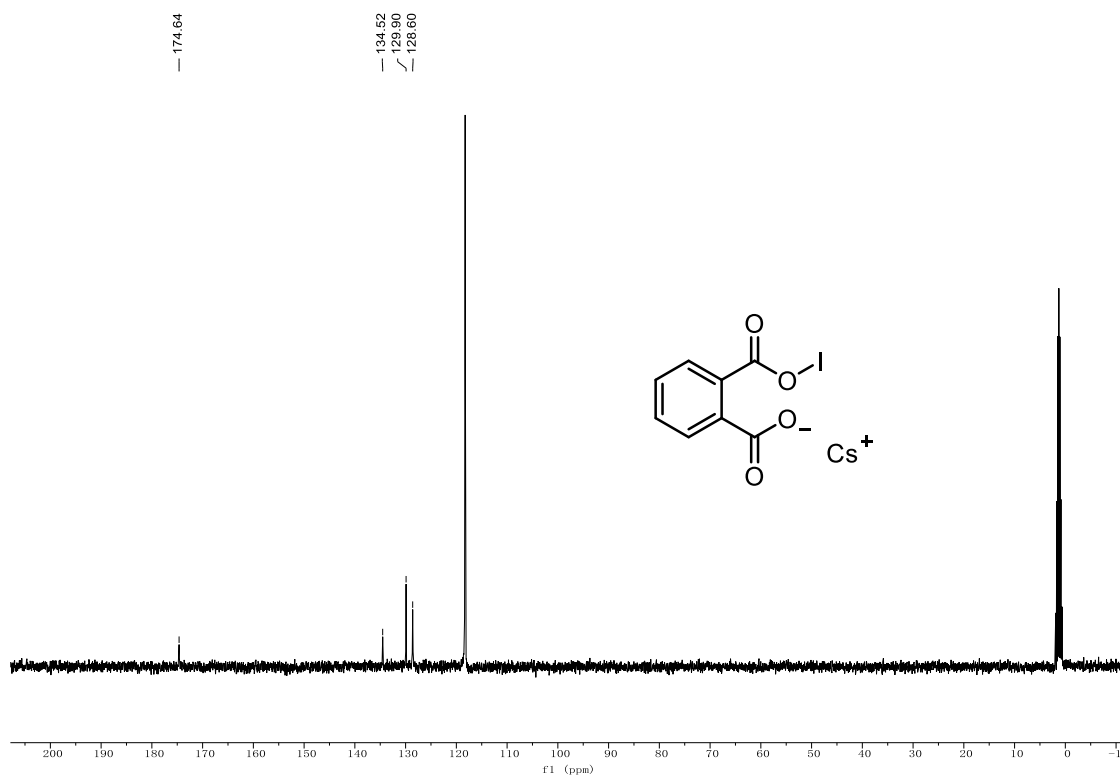
CsI (0.2 mmol, 1.0 equiv) was added to a 25 mL pressure tube under high vacuum with heating, and backfilled with N₂. CD₃CN (0.5 mL) were added under nitrogen atmosphere subsequently. PPO (0.2 mmol, 1.0 equiv) was added to the pressure tube in the end. The color of the solution is observed to be yellow, then stirred for 1h and the sample is taken for testing at this time.



BCTC-3

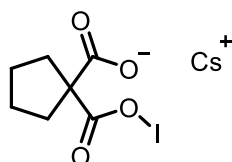
¹H NMR (400 MHz, CD₃CN) δ 7.48 – 7.38 (m, 2H), 7.37 – 7.27 (m, 2H). ¹³C NMR (101 MHz, CD₃CN) δ 174.64, 134.52, 129.90, 128.60.





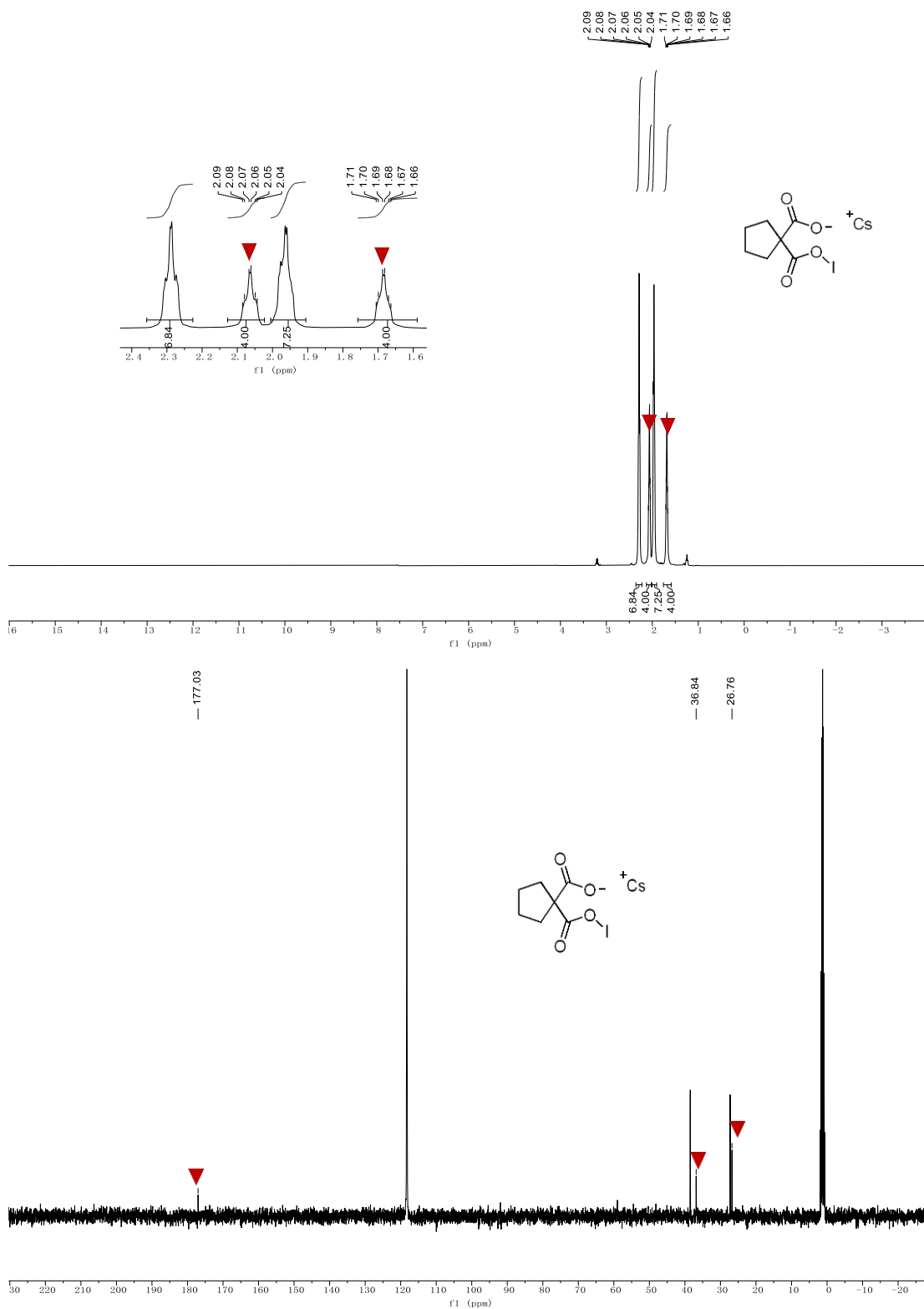
5.1.2 MPO + CsI

CsI (0.2 mmol, 1.0 equiv) was added to a 25 mL pressure tube under high vacuum with heating, and backfilled with N₂. CD₃CN (0.5 mL) were added under nitrogen atmosphere subsequently. MPO (0.2 mmol, 1.0 equiv) was added to the pressure tube in the end. The color of the solution is observed to be yellow, then stirred for 2h and the sample is taken for testing at this time. The red triangular symbols are labeled with the NMR peaks of the corresponding target compounds. The unlabeled NMR peaks are MPO.



BCTC-4

¹H NMR (400 MHz, CD₃CN) δ 2.06 (td, *J* = 7.2, 2.2 Hz, 4H), 1.68 (h, *J* = 2.5 Hz, 4H). ¹³C NMR (101 MHz, CD₃CN) δ 177.03, 36.84, 26.76.

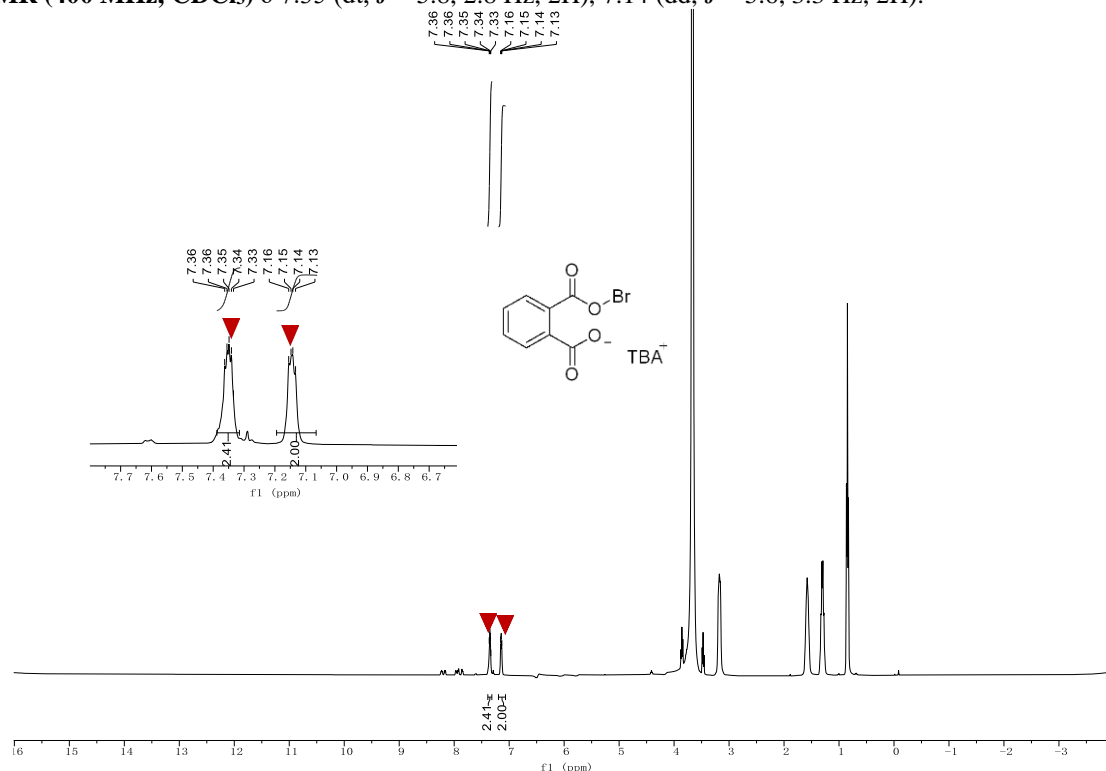


5.1.3 PPO + TBAB

TBAB (0.2 mmol, 1.0 equiv) was added to a 25 mL pressure tube under high vacuum with heating, and backfilled with N_2 . DCE (0.5 mL) were added under nitrogen atmosphere subsequently. PPO (0.2 mmol, 1.0 equiv) was added slowly in a glovebox under dark and a nitrogen atmosphere. The color of the

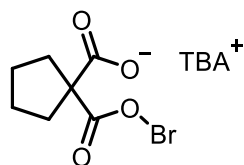
solution is observed to be pale chartreuse, and was added to CHCl_3 (0.5 mL). The sample is taken for testing during the 5 minutes. The red triangular symbols are labeled with the NMR peaks of the part of corresponding target compounds. The unlabeled NMR peaks are TBAB and solvent.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.35 (dt, $J = 5.8, 2.8$ Hz, 2H), 7.14 (dd, $J = 5.6, 3.3$ Hz, 2H).



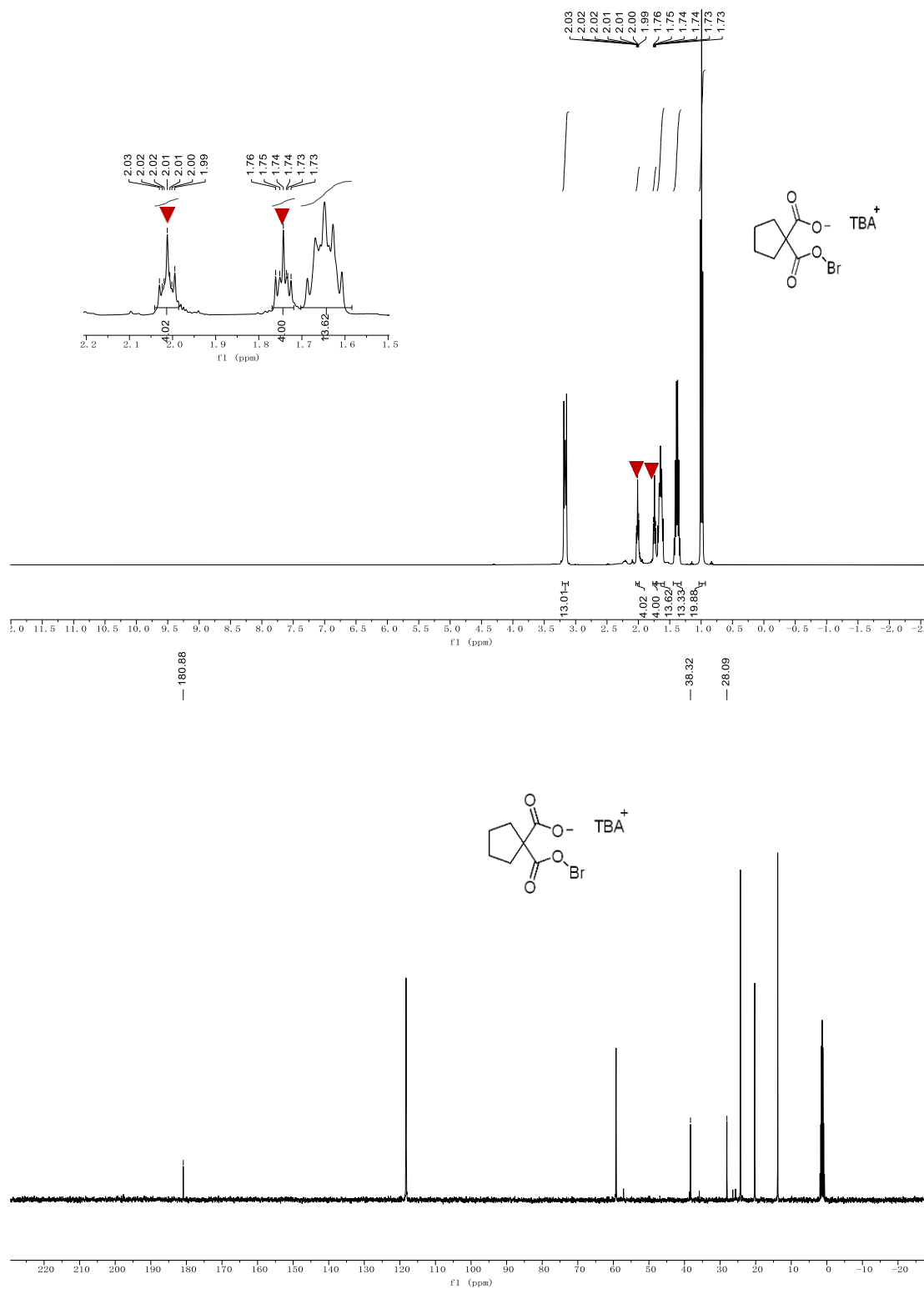
5.1.4 MPO + TBAB

TBAB (0.2 mmol, 1.0 equiv) was added to a 25 mL pressure tube under high vacuum with heating, and backfilled with N_2 . CD_3CN (0.5 mL) were added under nitrogen atmosphere subsequently. MPO (0.2 mmol, 1.0 equiv) was added slowly in a glovebox under dark and a nitrogen atmosphere. The color of the solution is observed to be pale chartreuse, and the sample is taken for testing during the 5 minutes. The red triangular symbols are labeled with the NMR peaks of the part of corresponding target compounds. The unlabeled NMR peaks are TBAB



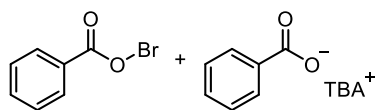
BCTC-2

$^1\text{H NMR}$ (400 MHz, CD_3CN) δ 2.05 – 1.97 (m, 4H), 1.84 – 1.71 (m, 4H). $^{13}\text{C NMR}$ (101 MHz, CD_3CN) δ 180.88, 38.32, 28.09.

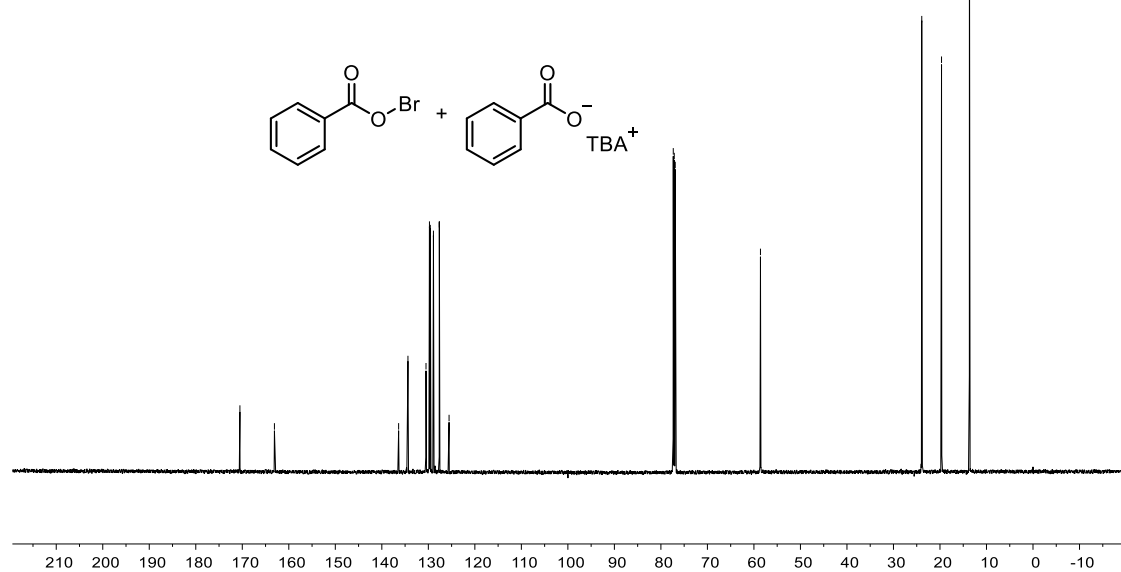
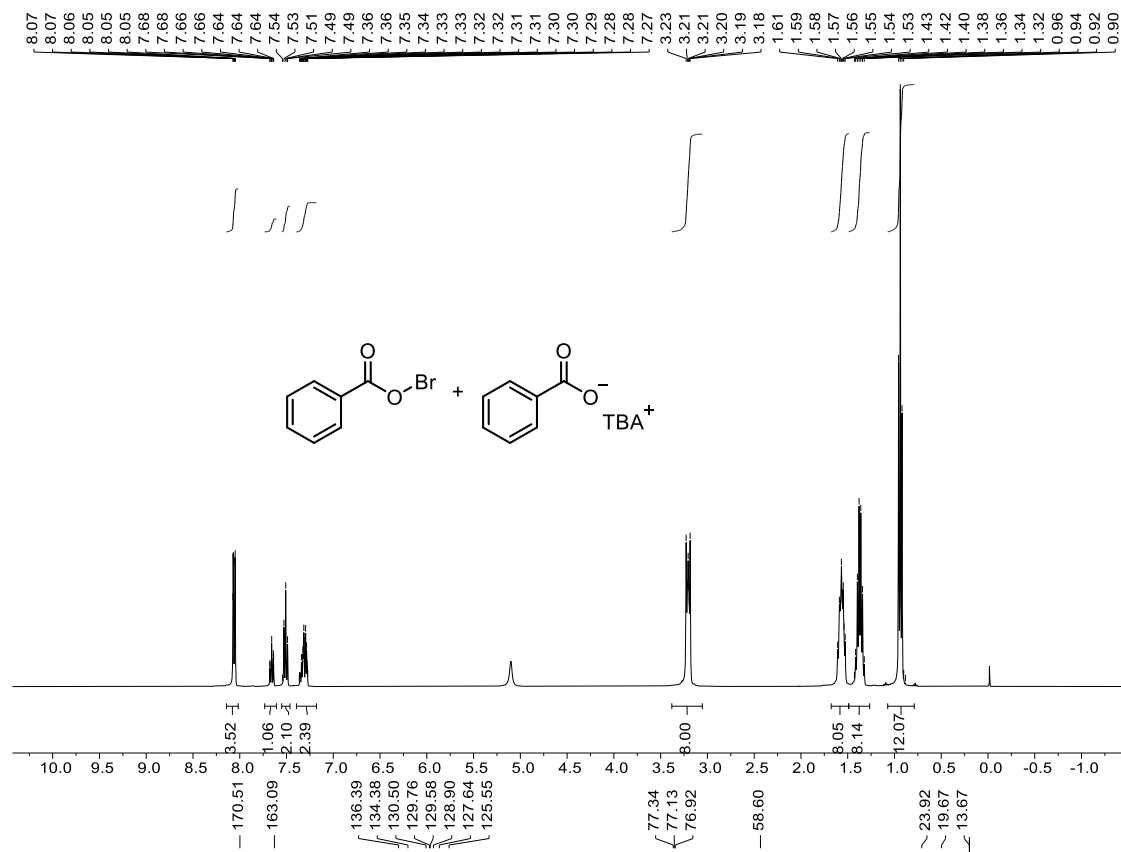


5.1.5 BPO + TBAB

TBAB (0.1 mmol, 1.0 equiv) was added to a 25 mL pressure tube under high vacuum with heating, and backfilled with N₂. CDCl₃ (0.5 mL) was added under nitrogen atmosphere subsequently. BPO (0.1 mmol, 1.0 equiv) was added slowly in a glovebox under dark and a nitrogen atmosphere

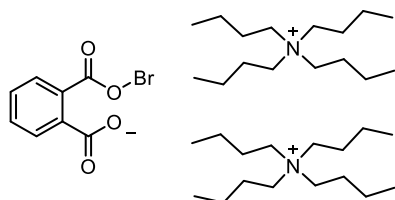


$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.18 – 7.97 (m, 4H), 7.69 – 7.59 (m, 1H), 7.51 (t, $J = 7.7$ Hz, 2H), 7.38 – 7.26 (m, 3H), 3.30 – 3.05 (m, 8H), 1.61 – 1.50 (m, 8H), 1.37 (h, $J = 7.3$ Hz, 8H), 0.94 (t, $J = 7.3$ Hz, 12H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 170.51, 163.09, 136.39, 134.38, 130.50, 129.76, 129.58, 128.90, 127.64, 125.55, 77.34, 77.13, 76.92, 58.60, 23.92, 19.67, 13.67.



5.2 Experiment data of HRMS about BCTC

TBAB (0.2 mmol, 1.0 equiv) was added to a 25 mL Schlenk tube under high vacuum with heating, and backfilled with N₂. MeCN (0.5 mL) were added under nitrogen atmosphere subsequently. PPO (0.2 mmol, 1.0 equiv) was added to the pressure tube in the end. The color of the solution is observed to be pale chartreuse, and the sample is taken for testing at this time.



HRMS (ES+) exact mass calculated for [M+H]⁺ (C₄₀H₇₆BrN₂O₄⁺) requires *m/z* 727.4983, found *m/z* 727.4982.

5.3 Experiment data of UV-Vis

UV spectra were recorded on shimadazu UV-2600.

5.3.1 PPO + TBAB

A solution of tetrabutylammonium bromide (TBAB) (16.1 mg, 0.05 mmol) in DCE (0.5 mL, in 5 mL volume of test vial), to which PPO (8.2mg, 0.05 mol) was added, was shaken. The reaction mixture was then diluted to 2.5×10^{-3} mol/L in carbon tetrachloride and drawn on the glass slide. Then UV spectra were measured. According to the Lambert-Beer law, the molar absorption coefficient was calculated:

$$\varepsilon = \frac{A}{cb} = \frac{1.871}{2.5 \times 10^{-3} \times 1} = 748.4 M^{-1}cm^{-1}$$

5.3.2 MPO + TBAB

A solution of TBAB (16.1 mg, 0.05 mmol) in DCE (0.5 mL, in 5 mL volume of test vial), to which MPO (7.8 mg, 0.05 mol) was added, was shaken. The reaction mixture was then diluted to 2.5×10^{-3} mol/L in carbon tetrachloride and drawn on the glass slide. Then UV spectra were measured. According to the Lambert-Beer law, the molar absorption coefficient was calculated:

$$\varepsilon = \frac{A}{cb} = \frac{1.981}{2.5 \times 10^{-3} \times 1} = 792.4 M^{-1}cm^{-1}$$

5.3.3 BPO + TBAB

A solution of TBAB (16.1 mg, 0.05 mmol) in DCE (0.5 mL, in 5 mL volume of test vial), to which BPO (12.1 mg, 0.05 mol) was added, was shaken. The reaction mixture was then diluted to 2.5×10^{-3} mol/L in carbon tetrachloride and drawn on the glass slide. Then UV spectra were measured.

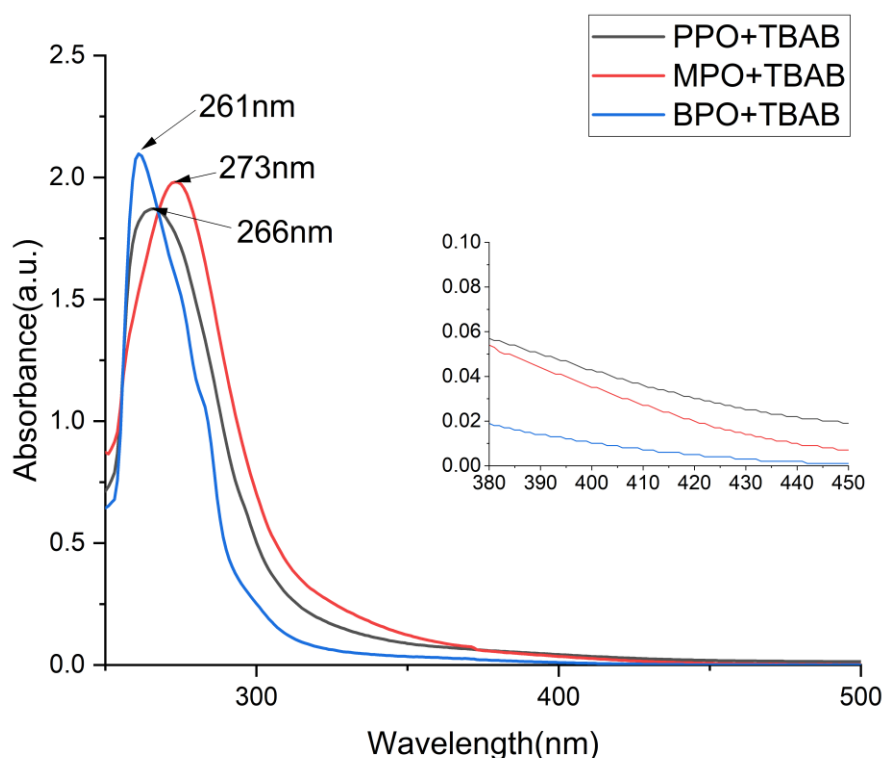


Figure S24. UV/Vis Experiment of PPO, MPO and BPO with TBAB

5.3.4 PPO + TBAB light

A solution of TBAB (16.1 mg, 0.05 mmol) in DCE (0.5 mL, in 5 mL volume of test vial), to which PPO (8.2mg, 0.05 mol) was added, was stirred for 2 h under blue LED. The reaction mixture was then diluted to 2.5×10^{-3} mol/L in carbon tetrachloride and drawn on the glass slide. Then UV spectra were measured.

Curve blue-shifted after illumination indicates that the mixture is degraded, which is consistent with the facts of the experiment. (Figure S25)

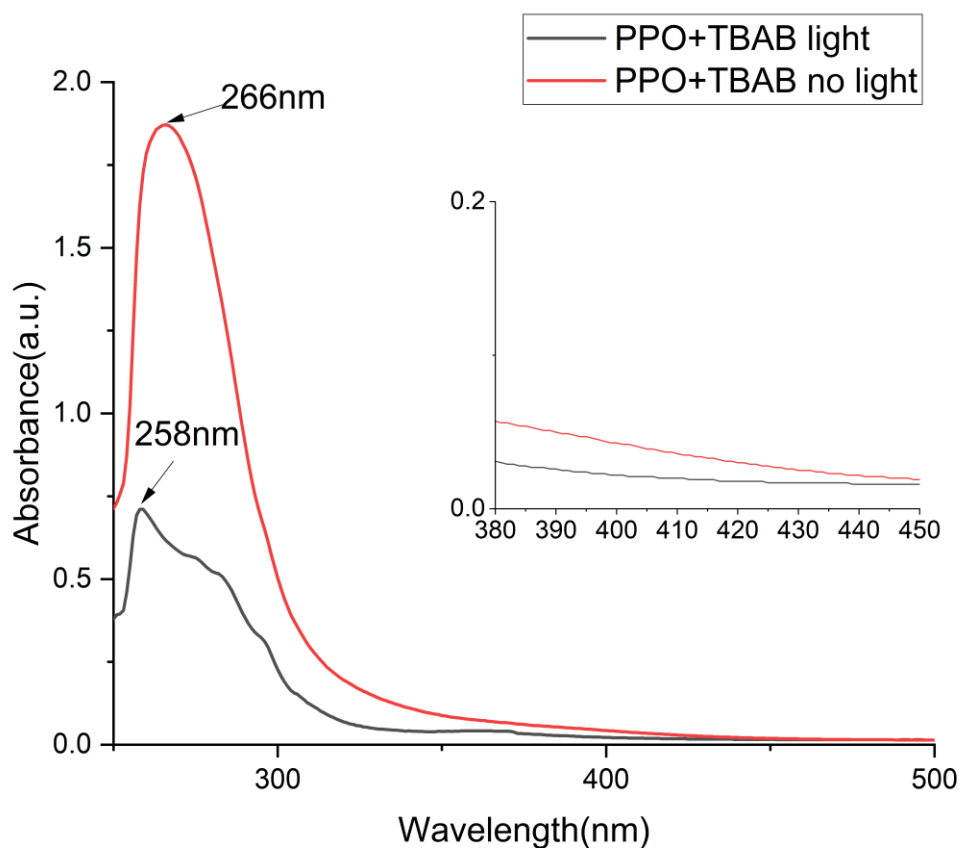


Figure S25. UV/Vis Experiment of PPO with TBAB under light or dark.

5.4 Experiment data of Raman

Raman spectra were recorded using Renishaw in Via Raman microscope equipped with thermoelectrically cooled CCD camera and fiber-optic cable for excitation and collection of Raman spectra. The 532-nm beam of the diode YAG laser was used as the excitation source. The laser power at the sample was about 1%. The laser beam was focused on a point in the reaction mixture on the glass slide.

5.4.1 TBAI + TBHP

First, the measurement was conducted under similar conditions with literature.^[30] A solution of tetrabutylammonium iodide (TBAI) (74 mg, 0.2 mmol) in CH₃CN (0.2 mL, in 5 mL volume of test vial), to which *tert*-butyl hydroperoxide (TBHP) (5.5 M in decane, 0.73 mL, 4 mmol) was added at 25 °C, was stirred for 2 h. The reaction mixture was then drawn on the glass slide and the Raman spectra were measured

5.4.2 BPO + TBAI

A solution of tetrabutylammonium iodide (TBAI) (74 mg, 0.2 mmol) in CH₃CN (1 mL, in 5 mL volume of test vial), to which BPO (48mg, 0.2 mol) was added at 25 °C, was stirred for 10 min. The reaction mixture was then drawn on the glass slide and the Raman spectra were measured.

5.4.3 BPO + CsI

A solution of CsI (52 mg, 0.2 mmol) in CH₃CN (1 mL, in 5 mL volume of test vial), to which BPO (48mg, 0.2 mol) was added at 25 °C, was stirred for 2 h. The reaction mixture was then drawn on the glass slide and the Raman spectra were measured.

5.4.4 MPO + TBAI

A solution of TBAI (74 mg, 0.2 mmol) in CH₃CN (1 mL, in 5 mL volume of test vial), to which MPO (31mg, 0.2 mol) was added at 25 °C, was stirred for 10 min. The reaction mixture was then drawn on the glass slide and the Raman spectra were measured.

5.4.5 MPO + CsI

A solution of CsI (52 mg, 0.2 mmol) in CH₃CN (1 mL, in 5 mL volume of test vial), to which MPO (31 mg, 0.2 mmol) was added at 25 °C, was stirred for 2 h. The reaction mixture was then drawn on the glass slide and the Raman spectra were measured.

5.4.6 PPO + CsI

A solution of CsI (52 mg, 0.2 mmol) in CH₃CN (1 mL, in 5 mL volume of test vial), to which PPO (33 mg, 0.2 mmol) was added at 25 °C, was stirred for 2 h. The reaction mixture was then drawn on the glass slide and the Raman spectra were measured.

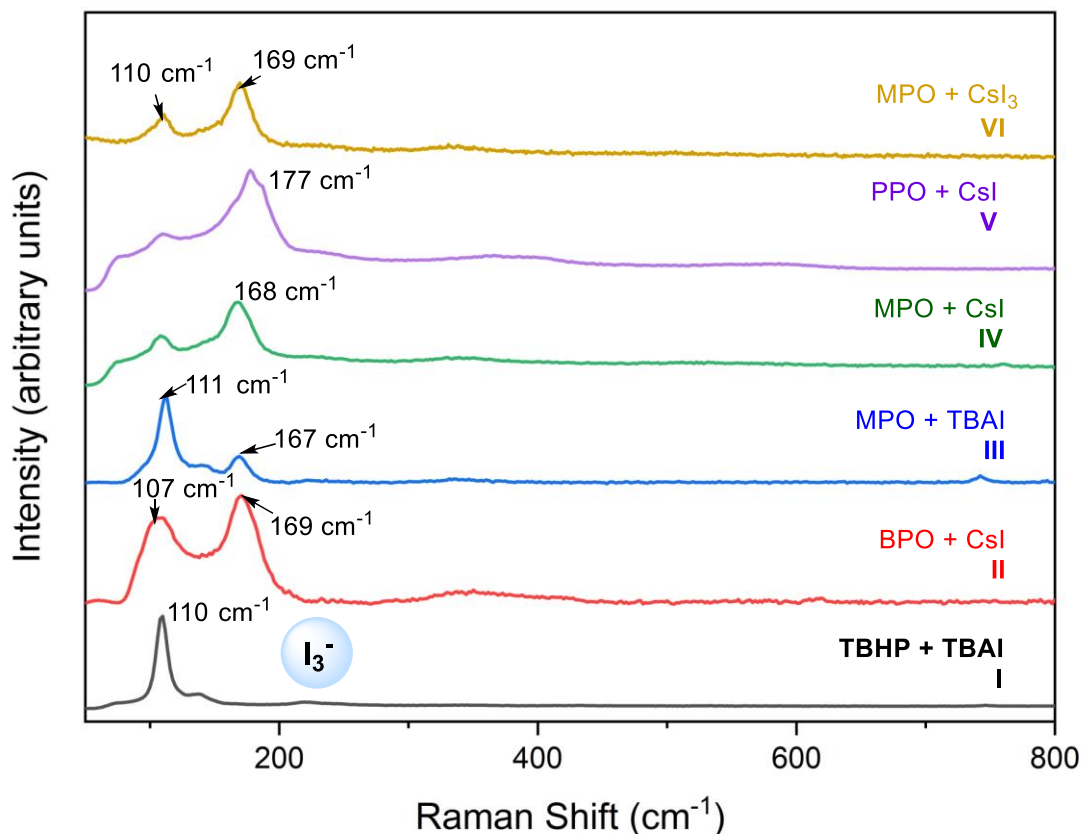


Figure S26. Raman spectra of oxidants and iodine source

The bands at 110 cm^{-1} were assigned to triiodide (I_3^-) according the literature⁴⁵. The combination of TBAI and TBHP (**Figure S26**, spectrum **I**) was used as a referenced I_3^- system. Obviously, there are also I_3^- in other four spectrums **II** to **VI** of iodine source and oxidants. In addition, the higher peaks in spectrums **V** to **VI** were supposed as corresponding acyl hypoiodite ($\text{R-CO}_2\text{I}$). Compared with BPO system (**Figure S26**, spectrums **II** and **III**), the cyclic diacyl peroxide systems (**Figure S26**, spectrums **IV** to **V**) were neater (the peaks corresponding acyl hypoiodite was more visible). Compared with TBAI and CsI (**Figure S26**, spectrums **II** and **III** or **IV** and **V**), acyl hypoiodite ($\text{R-CO}_2\text{I}$) were more easily generated in CsI system.

5.5 Optimization of BCTC-induced reactions

Table S8 Screening of the optimal oxidant in ring-opening halogenation of cycloalkanols^a

Ring opening of cycloalkanols

Org. Lett. **2018**, 20(4), 1228-1231.

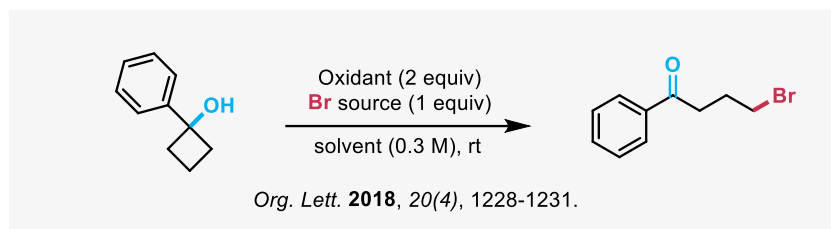
PPO-1
MPO-1
BPO
H₂O₂
t-Bu-O-O-H
CHP

Entry	Oxidant	Br source	Light	Solvent	Time	Yield ^b [%]
1	PPO-1	TBAB	Blue LED	DCE	30 min	95
2	MPO-1	TBAB	Blue LED	DCE	30 min	94
3	BPO	TBAB	Blue LED	DCE	12 h	20
4	H ₂ O ₂	TBAB	Blue LED	DCE	12 h	NR
5	TBHP	TBAB	Blue LED	DCE	12 h	trace
6	CHP	TBAB	Blue LED	DCE	12 h	NR
7	<i>m</i> -CPBA	TBAB	Blue LED	DCE	12 h	84
8	LPO	TBAB	Blue LED	DCE	12 h	23
9	DTBP	TBAB	Blue LED	DCE	12 h	35
10	Dicumyl Peroxide	TBAB	Blue LED	DCE	12 h	NR
11	PPO	TBAB	None	DCE	12 h	59

[a] Reaction conditions: **1a** (0.1 mmol, 1 equiv.), oxidant (0.2 mmol, 2.0 equiv.), TBAB (0.1 mmol, 1.0 equiv.), and DCE (1 mL), blue LED, r.t; [b] Yields of isolated products.

Table S9 Screening of the different alkali metal ions in ring-opening halogenation of cycloalkanols^a

Ring opening of cycloalkanols

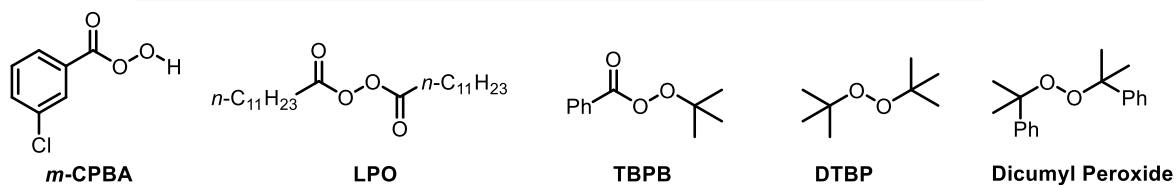
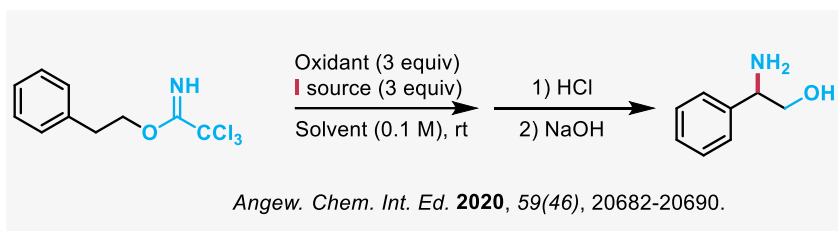


Entry	Oxidant	Br source	Light	Solvent	Time	Yield ^b [%]
1	PPO-1	TBAB	Blue LED	DCE	30 min	95
2	PPO-1	NBS	Blue LED	DCE	12 h	NR
3	PPO-1	CsBr	Blue LED	DCE	12 h	NR
4	PPO-1	KBr	Blue LED	DCE	12 h	NR
5	PPO-1	NaBr	Blue LED	DCE	12 h	NR

[a] Reaction conditions: **1a** (0.1 mmol, 1 equiv.), oxidant (0.2 mmol, 2.0 equiv.), TBAB (0.1 mmol, 1.0 equiv.), and DCE (1 mL), blue LED, r.t.; [b] Yields of isolated products.

Table S10 Screening of the optimal oxidant in C(sp³)-H amination of imidates^a

C(sp³)-H aminations of imidates

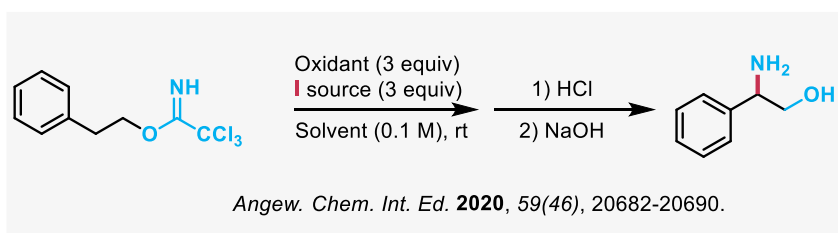


Entry	Oxidant	I source	Light	Solvent	Time	Yield ^b [%]
1	PPO-1	CsI	Sunlight	MeCN	2 h	93
2	MPO-1	CsI	sunlight	MeCN	2 h	93
3	BPO	CsI	sunlight	MeCN	8 h	34
4	H ₂ O ₂	CsI	Blue LED	MeCN	8 h	trace
5	TBHP	CsI	Blue LED	MeCN	8 h	trace
6	CHP	CsI	Blue LED	MeCN	8 h	28
7	<i>m</i> -CPBA	CsI	Blue LED	MeCN	8 h	NR
8	LPO	CsI	Blue LED	MeCN	8 h	36
9	DTBP	CsI	Blue LED	MeCN	8 h	40
10	Dicumyl Peroxide	CsI	Blue LED	MeCN	8 h	61
11	PPO	CsI	None	MeCN	8 h	trace

[a] Reaction conditions: **3a** (0.1 mmol, 1 equiv.), oxidant (0.3 mmol, 3.0 equiv.), CsI (0.3 mmol, 3.0 equiv.), and MeCN (2 mL), r.t; [b] Yields of isolated products.

Table S11 Screening of the different alkali metal ions in C(sp³)-H amination of imidates^a

C(sp³)-H aminations of imidates



Entry	Oxidant	I source	Light	Solvent	Time	Yield ^b [%]
1	PPO-1	CsI	Sunlight	MeCN	2 h	93
2	PPO-1	KI	sunlight	MeCN	2 h	49
3	PPO-1	LiI	sunlight	MeCN	2 h	34
4	PPO-1	NaI	sunlight	MeCN	2 h	59
5	PPO-1	TBAI	sunlight	MeCN	2 h	trace

[a] Reaction conditions: **1a** (0.1 mmol, 1 equiv.), oxidant (0.2 mmol, 2.0 equiv.), TBAB (0.1 mmol, 1.0 equiv.), and DCE (1 mL), blue LED, r.t; [b] Yields of isolated products.

5.6 Higher energy light for the photochemical homolyses of the O–I bond

The higher BDE of O–I bonds of the acyl hypoiodite (R–CO₂I) generated from BPO was provided in Figure S (BDE = 33.3 kcal/mol = 139.42 kJ/mol). Based on the Planck–Einstein relation ($E = h\nu = \frac{hc}{\lambda}$), the approximate wavelength in theory was estimated as 858 nm (Equation 1).

$$\lambda = \frac{N_0 hc}{E} = \frac{6.023 \times 10^{23} \times 6.6256 \times 10^{-34} \times 2.998 \times 10^8}{139.42 \times 10^{-9} \times 10^3} = 858 \text{ nm} \quad (1)$$

In consideration of the illumination efficiency and other factors, such as the likely steric effect, we chose the 300 nm light as the illumination condition and BPO as the oxidant to perform the C(sp³)–H amination reaction and ring-opening halogenation reaction.

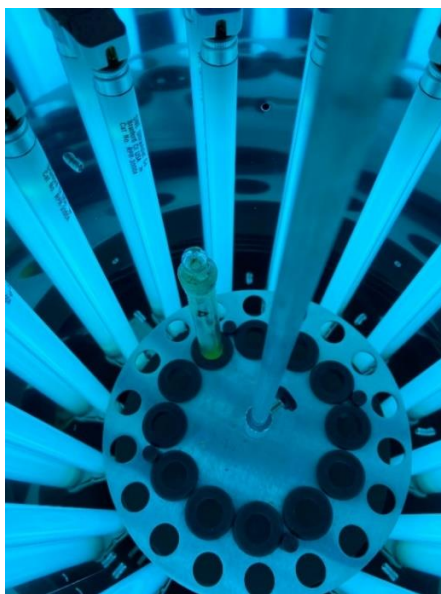
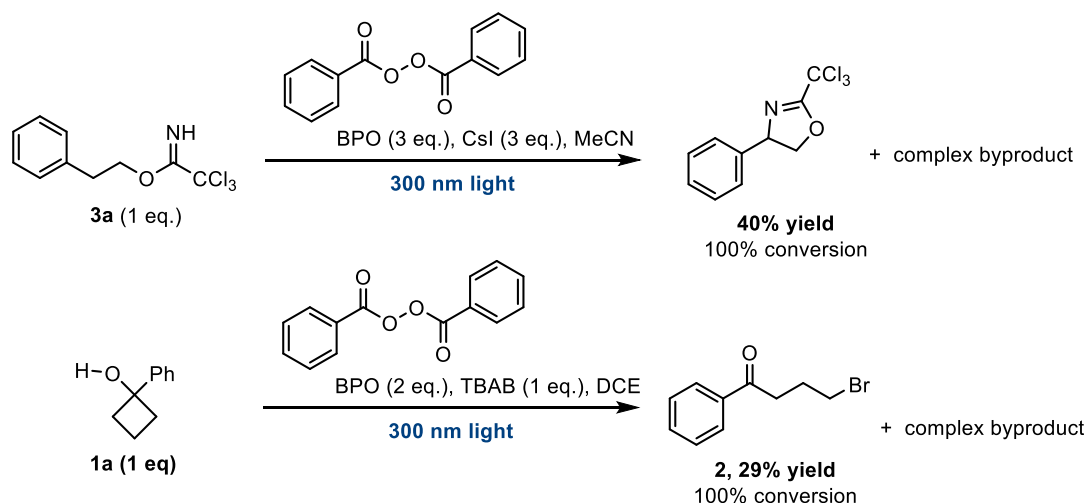


Figure S27. The instrument of 300 nm illumination condition



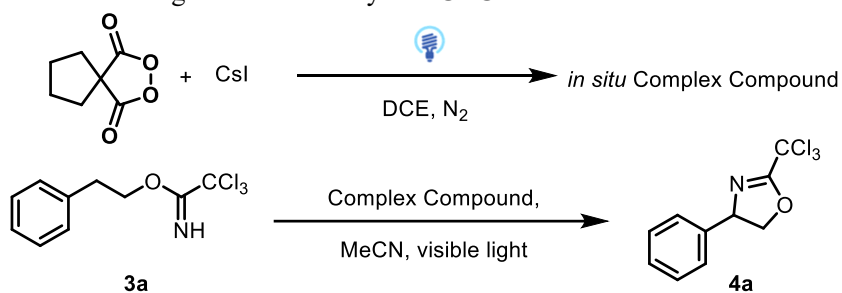
Scheme S1. Experimental results of BPO with higher energy light

Finally, 40% yield of oxazoline product and 29% yield of bromination linear ketone were isolated with no significant improvement in yields compared with 34% yield and 20% yield (**Scheme S1**). The quite higher energy light does not bring significant improvement in yields, suggesting that the efficiency of generating

acyloxy radicals is not a restrictive factor. The low yield of oxazoline and bromination linear ketone accurately reflects the relatively poor reactivity of BPO, and the intramolecular base brought by the cyclic structure of peroxides indeed plays a key role in this transformation.

5.7 The influence of light on the stability of BCTC

Table S12. The influence of light on the stability of **BCTC-4**

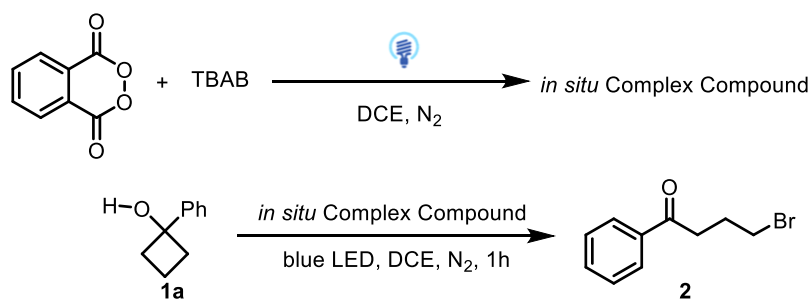


Entry	Conditions before substrates added	Yield
1	MPO+CsI under blue LED 30 min	89%
2	MPO+CsI under blue LED 60 min	82%
3	MPO+CsI under dark 30 min	88%

Experiments procedures:

In a reaction vial, CsI (33 mg, 0.1 mmol, 1.0 equiv.) in dry MeCN (0.5 mL) was added MPO (15 mg, 0.1 mmol, 1.0 equiv.). The mixture was stirred for 30 minutes, and 60 minutes under blue LED and 30 minutes under dark. Then the substrate was added. The desired product could be obtained in 89% yield in the **entry 1** and 82% yield in the **entry 2**, while in 88% yield in the **entry 3**.

Table S13. The influence of light on the stability of **BCTC-1**



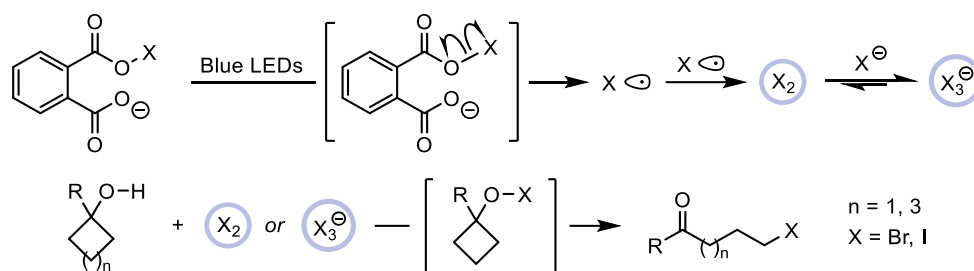
Entry	Conditions before substrates added	Yield
1	PPO+TBAB under blue LED 30 min	12%
2	PPO+TBAB under blue LED 60 min	trace
3	PPO+TBAB under dark 30 min	24%

Experiments procedures:

In a reaction vial, TBAB (33 mg, 0.1 mmol, 1.0 equiv.) in dry DCE (0.5 mL) was added PPO (16 mg, 0.1 mmol, 1.0 equiv.). The mixture was stirred for 30 minutes, and 60 minutes under blue LED and 30 minutes under dark. Then the substrate was added. The desired product could be obtained in 12% yield in the **entry 1** and trace yield in the **entry 2**, while in 24% yield in the **entry 3**.

5.8 NMR evidence for excluding the formation of X_2 or $TBAX_3$ ($X = Br$)

In the previous section, we confirmed that the reaction between intermediate **BCTC** and cycloalkanols **1b** provides trace amount of hypobromite in the absence of light. Mechanically, however, the weak O–X bond ($X = Br, I$) of intermediate **BCTC** could undergo homolysis and generate the corresponding halogen radical under the irradiation of visible light, which is capable to subsequently capturing another halogen radical via radical-radical coupling to afford X_2 . Furthermore, in the presence of excess X^- , the in-situ generated X_2 forms X_3^- due to a Lewis acid/base interaction between X_2 and X^- . Based on previous studies reported by Nagib, the visible-light-promoted halogenation of cycloalkanols **1** by X_2 or X_3^- seems a possible way to afford corresponding ring-opening products.



Scheme S2. Possible mechanism for X_2 or X_3^- -induced ring-opening halogenation

From this point of view, in order to verify whether this pathway represents the major pathway of this reaction, we operated the reaction system between cycloalkanols and Br_2 , $TBABr_3$, I_2 and $TBAI_3$, respectively. In addition, tetrabutylammonium benzoate was added as Brønsted base to minimize the differences between the mechanism investigation experiments and the reaction system of PPO-induced ring-opening halogenation. A series of NMR studies are presented as follows:

5.8.1. ^{13}C NMR characterization of visible-light-promoted Br_2 -induced ring-opening bromination of **1a**:

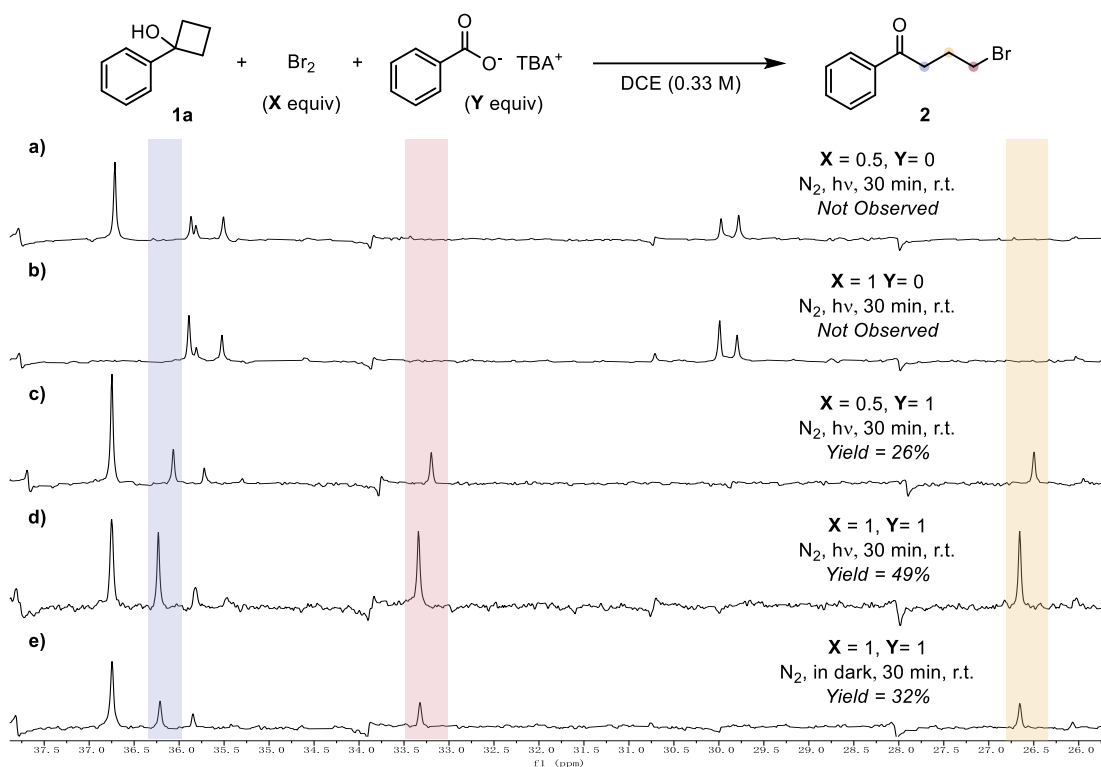
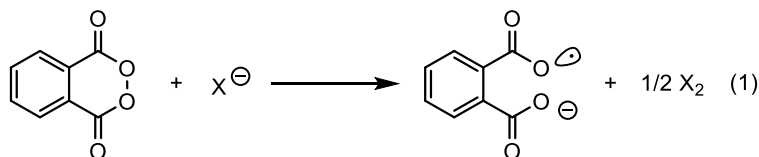


Figure S28. ^{13}C NMR characterization of visible-light-promoted Br_2 -induced ring-opening bromination of 1-phenylcyclobutan-1-ol **1a**



According to equation (1), while 1 equivalent of TBAX was to the reaction system, up to 0.5 equivalent of X_2 can be produced during the reaction. Hence, the reaction between 0.5 equivalent Br_2 and 1 equivalent of **1a** was performed initially. Nevertheless, unidentified by-products were obtained instead of desired product (**Figure S28, a**), and the addition of more Br_2 only lead to a total consumption of starting material and an increase in by-products (**Figure S28, b**).

Intriguing, due to the intermolecular hydrogen-bond interaction, the desired product could be obtained in 26% yield in the participation of 1 equivalent of Brønsted base (**Figure S28, c**). Added an excessive equivalent of Br_2 only afford a reasonable increase in the yield of **2** from 26% to 49% (**Figure S28, d**). Compared with our published data, the relative low yield indicated the Br_2 -induced ring-opening bromination is not the main pathway even a 100% conversion from TBAB to Br_2 was happened. Namely, the covalently tethered distonic radical anions play a significant role during the generation of desired product.

In the previous section, the polar pathway without the participation of visible light has been excluded, the homolysis of weak O–Br bond in **BCTC** was not under consideration. In another words, we defaulted that the O–Br bond in **BCTC** undergo heterolysis in the absence of visible light. In this part, the assessment of the contribution of visible light in the process of reaction is applicable. It is worthy mentioned that,

although we have excluded the Br₂-induced ring-opening bromination pathway, herein we still assume that Br₂ represents the key bromination reagent for more rigorous contrast. As described before, the generation of Br₂ could not be realized without the participation of visible light, however, whether the visible light is necessary for the formation of hypobromites too? Take the advantage of that the C–C cleavage of **2** occurs too fast to detect and could afford the desired product **2** immediately even in dark, we operated the visible light control experiment to value the contribution of visible light to answer this question. Ultimately, **2** could be obtained in a yield of 32% (**Figure S28, e**), the result of which suggested that although the visible light does promote the formation of hypobromite, it is not necessary for this process.

5.8.2. ¹³C NMR characterization of visible-light-promoted TBABr₃-induced ring-opening bromination of **1c**:

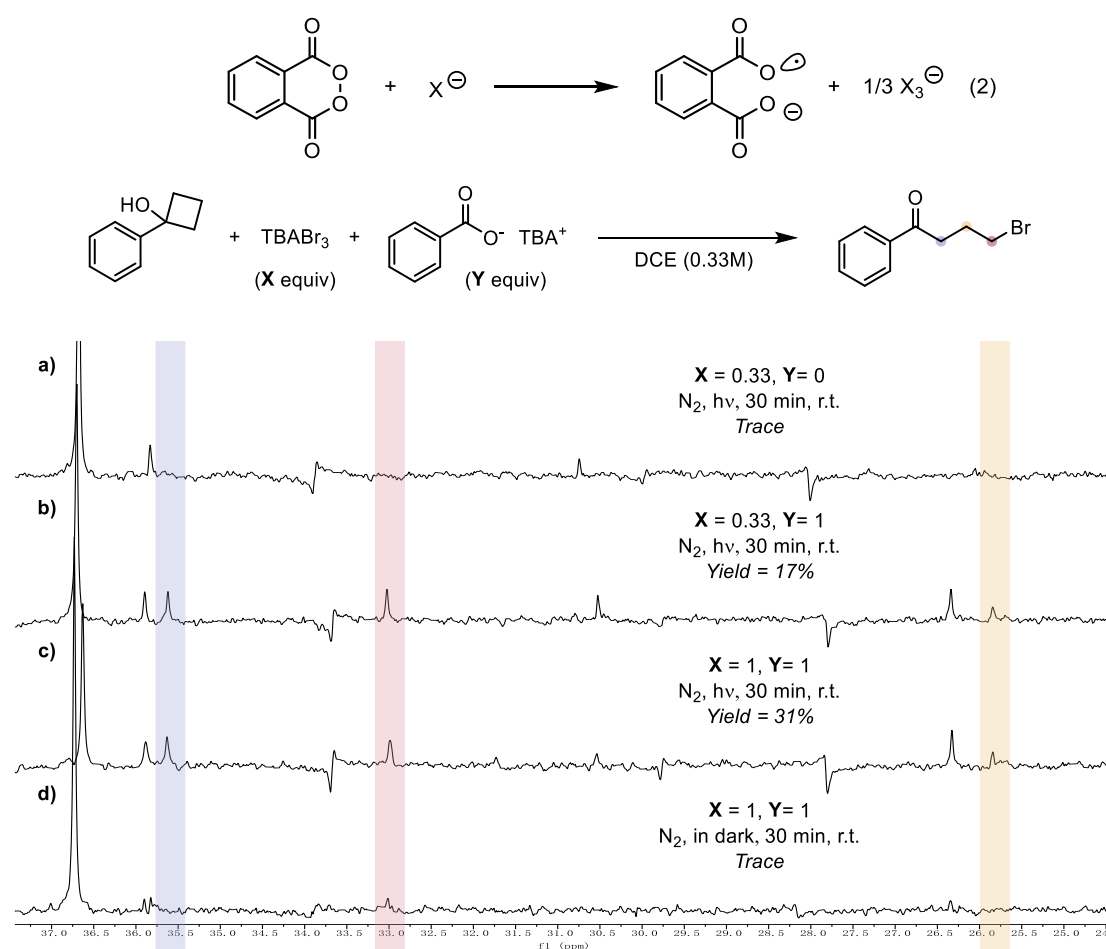


Figure S29. ¹³C NMR characterization of visible-light-promoted TBABr₃-induced ring-opening bromination of 1-phenylcyclobutan-1-ol **1a**

According to equation (2), while 1 equivalent of TBAX was to the reaction system, up to 0.33 equivalent of X₃[⊖] can be produced during the reaction. Similar results were observed when 0.33 equivalent and 1 equivalent tetrabutylammonium tribromide (TBABr₃) was employed as bromination reagent. First of all, the reaction of only TBABr₃ and **1a** afforded no desired product **2** (**Figure S29, a**). Subsequently, added

tetrabutylammonium benzoate as Brønsted base and increase the equivalent of TBABr₃ in reaction system led to the generation of **2** in the yield of 17% and 31% (**Figure S29, b and c**), respectively. Again, compared with our published data, the relative low yield indicated the TBABr₃-induced ring-opening bromination is also not the main pathway even a 100% conversion from TBAB to TBABr₃ was happened. Interestingly, the ¹³C NMR study of the visible light control experiment shows that no desired product was formed in dark even in the presence of 1 equivalent of tetrabutylammonium benzoate, the result of which indicate visible light plays a critical role in both the homolysis of O–Br bond in **BCTC** and the formation of corresponding hypobromite (**Figure S29, d**).

5.8.3. ¹³C NMR characterization of visible-light-promoted TBABr₃-induced ring-opening bromination of **1b**:

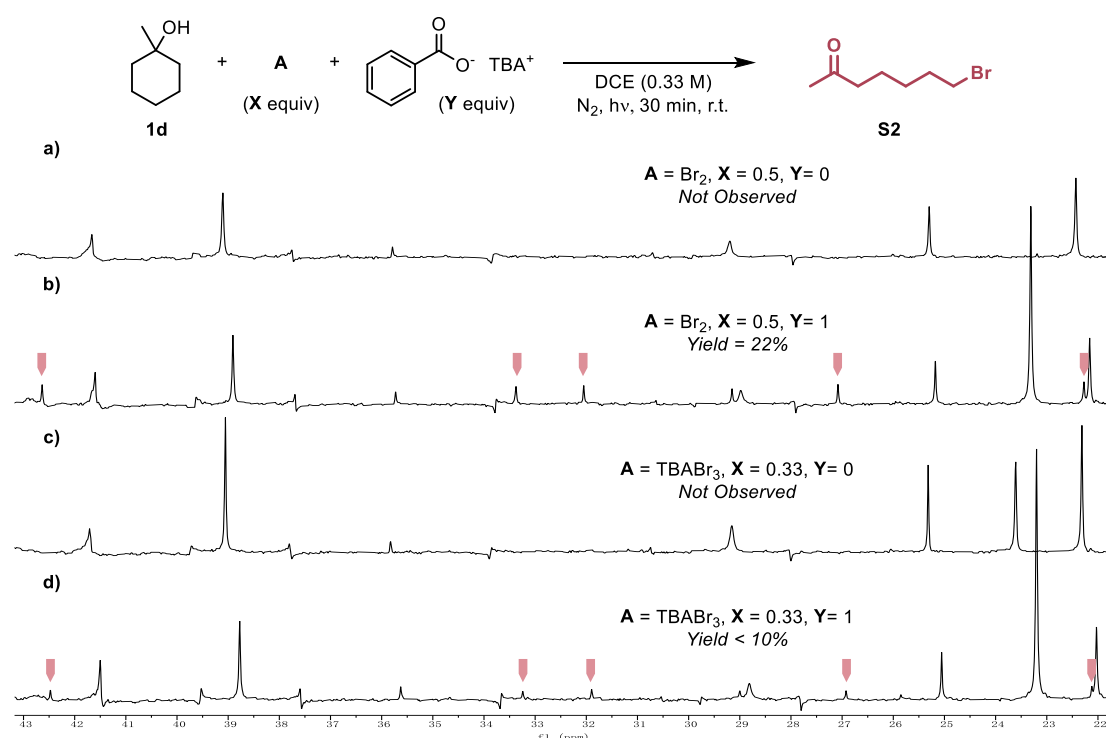
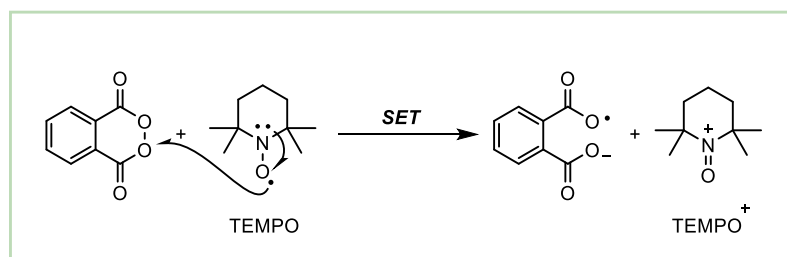


Figure S30. ¹³C NMR characterization of visible-light-promoted TBABr₃-induced ring-opening bromination of **1d**

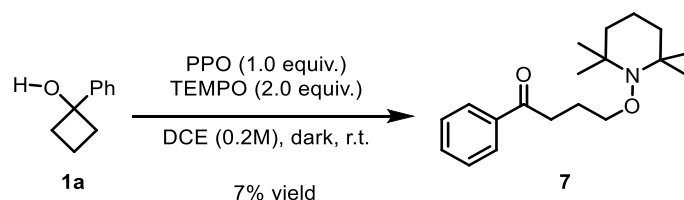
Take account of the possible different ring-opening pathway for four- and six-membered cycloalkanols (concerted mechanism and stepwise mechanism), the Br₂- and TBABr₃-induced ring-opening bromination of **1d** were also performed as supplement. Although slight decline in the yield of corresponding product were observed, the trend was consistent with the experiment results demonstrated above.

6. Designed polarity matching experiment



Scheme S3 PPO-TEMPO adduct

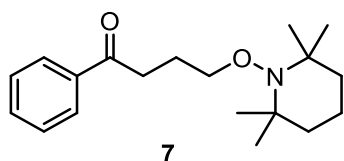
As shown in the previous report, in the reaction of ring-opening halogenation of cycloalkanols, when the TBAB was excluded from the reaction system, the PPO-induced ring-opening cycloalkanols could not proceed smoothly. While TEMPO is highly effective as an inhibitor of aerobic oxidations, its one-electron oxidation with, for example, chlorine or bromine, results in the formation of the corresponding oxoammonium cation, which serves as a relatively potent oxidant and is capable of generating TRDA-5. Thus, 1 equivalent of TEMPO was added instead of TBAB, and to our delight the ring-opening cycloalkanols addition product **7** was isolated albeit in a low yield (7%). This encouraging experimental result revealed that the identical product obtained when employing TEMPO under halogen-free conditions has confirmed that the ring-opening reaction of cycloalkanols, as initially reported, can be achieved without the presence of halogens. Moreover, to give more comprehensive evidence of the significant role of the radical anion played in cleavage of the N–H, we carried out the cyclization of thiobenzanilides experiment under the guidance of polarity umpolung strategy in which the cyclization product was isolated in a good yield (80%), using 1.5 equivalent TEMPO and 2.0 equivalent PPO under the dark condition. In addition, there are no cyclization product under same condition without PPO.



Scheme S4. Experiments of PPO and TEMPO in the ring-opening halogenation of cycloalkanols

Experiments procedures:

In a reaction vial, TEMPO (0.2 mmol, 2.0 equiv.) in dry DCE (0.5 mL) was added PPO (0.1 mmol, 1.0 equiv.) and the substrate (0.1 mmol, 1.0 equiv.). The mixture was stirred for 60 minutes under dark condition. The desired product could be obtained in 7% isolated yield

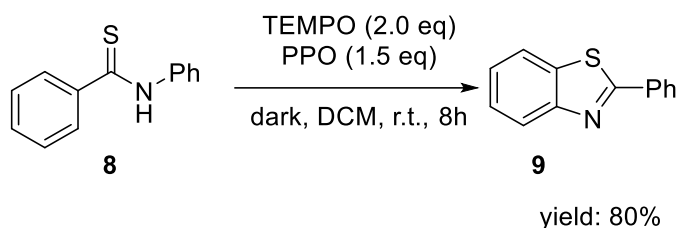


$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.98 (dd, $J = 7.2, 1.8$ Hz, 2H), 7.60 – 7.52 (m, 1H), 7.46 (t, $J = 7.6$ Hz, 2H), 3.83 (t, $J = 6.2$ Hz, 2H), 3.10 (t, $J = 7.5$ Hz, 2H), 1.98 (p, $J = 6.6$ Hz, 2H), 1.44 (dd, $J = 8.4, 4.8$ Hz, 4H), 1.37 – 1.22

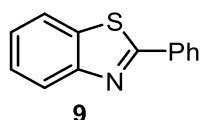
(m, 2H), 1.15 (s, 6H), 1.09 (s, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 200.35, 137.15, 133.05, 128.70, 128.20, 75.63, 59.85, 39.70, 35.62, 33.21, 23.76, 20.24, 17.24.

These data are consistent with that previously reported.⁴⁶

In a reaction vial, TEMPO (0.2 mmol, 2.0 equiv.) in dry DCM (0.5 mL) was added PPO (0.15 mmol, 1.5 equiv.) and the substrate (0.1 mmol, 1.0 equiv.). The mixture was stirred for 8h under dark. The desired product could be obtained in 85% isolated yield



Scheme S5. Experiments of PPO and TEMPO in the cyclization of thiobenzanilides



^1H NMR (400 MHz, CDCl_3) δ 8.09 (ddd, $J = 7.8, 5.2, 2.3$ Hz, 3H), 7.91 (dd, $J = 8.0, 1.2$ Hz, 1H), 7.50 (tt, $J = 4.9, 2.6$ Hz, 4H), 7.39 (td, $J = 7.6, 1.2$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 168.23, 154.25, 135.18, 133.72, 131.12, 129.16, 127.69, 126.46, 125.33, 123.35, 121.76.

These data are consistent with that previously reported.⁴⁷

7. Computational studies of BCTC

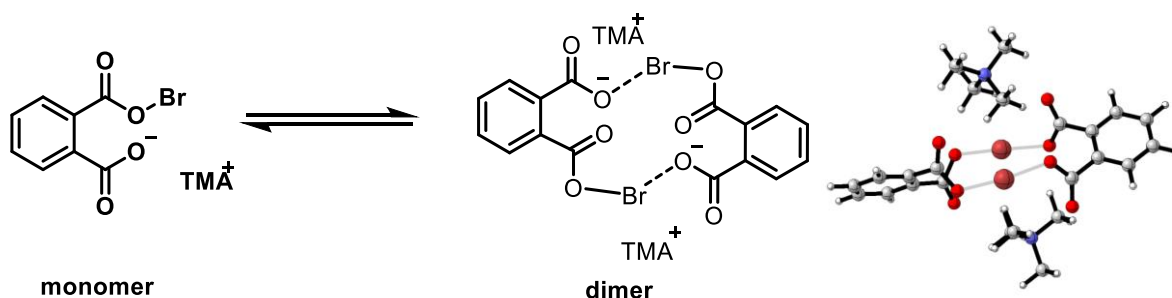
7.1 Computational Methods

All DFT calculations were performed using Gaussian suite of programs.⁴⁸ For potential energy surface calculation, geometries of all species were fully optimized using B3LYP functional⁴⁹⁻⁵³ with GD3 dispersion correction⁵⁴ and 6-31+G(d) basis set. Solvent effects were considered by self-consistent reaction field (SCRF) using SMD model⁵⁵ during the geometry optimization with 1,2-dichloroethane or acetonitrile as a solvent. The solvation free energy, is calculated by subtracting the single point energy calculated under the solvent model from the single point energy calculated under the gas phase using M052x functional and 6-31G(d) basis set.⁵⁶ Vibrational frequencies calculations at the same level of theory were computed to ensure that either a minimum (for intermediates) or a first-order saddle point (for transition states) was obtained. More accurate electronic energies were calculated using B3LYP-D3/6-311++G(d,p) method in 1,2-dichloroethane or acetonitrile solvent. Unless otherwise specifies, the energies reported are Gibbs free energies under 298.15 K and 1 atm with solvent effect corrections. We also calculated homolytic bond dissociation enthalpies (BDE) for a number of molecules by using B3LYP-D3/6-311++G(d,p). The 3D structures of intermediates and transition states were illustrated using the CYLview software.⁵⁷

7.2 UV spectrum prediction by DFT.

UV spectrum were also calculated using TDDFT (B3LYP/6-311++G(d,p)/PCM (1,2-dichloroethane). The relevant UV/Vis wavenumbers for dimer are 261 nm, respectively, very close to our experimental observation. The computed UV-vis spectrum of the dimer demonstrates that the strong absorption at 261 nm is in good agreement with the experiment, whereas the monomer INT2B exhibits a peak at 210 nm (**Figure S31**).

7.2.1 PPO + TBAB



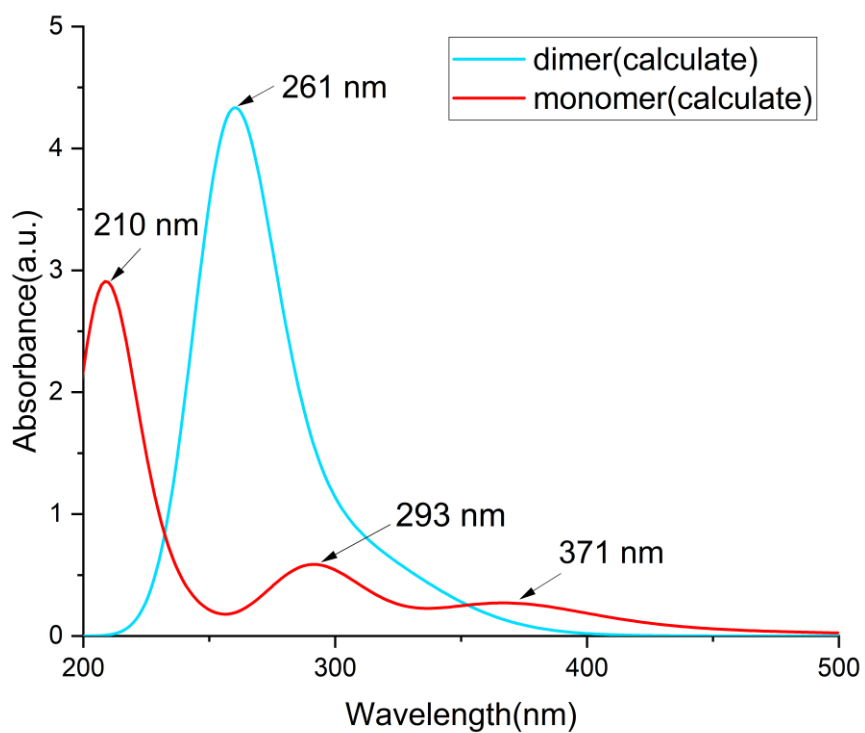
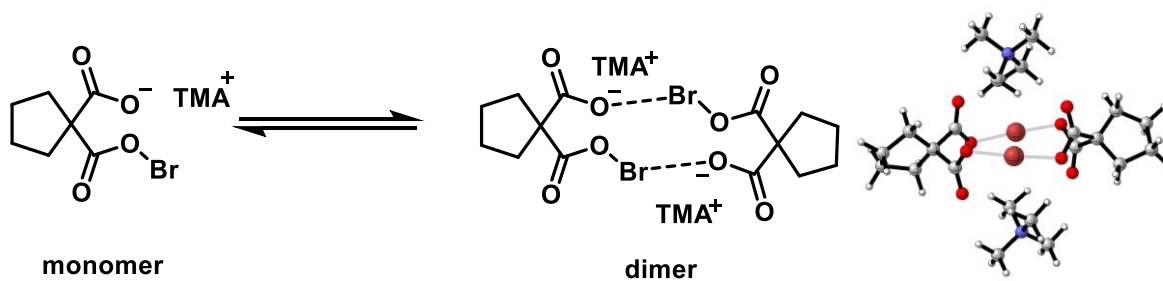


Figure S31. UV/Vis of PPO dimer and monomer (with TBAB) computed by TDDFT

7.2.2. MPO + TBAB



The relevant UV/Vis wavenumbers for dimer are 239 nm, respectively, very close to our experimental observation.

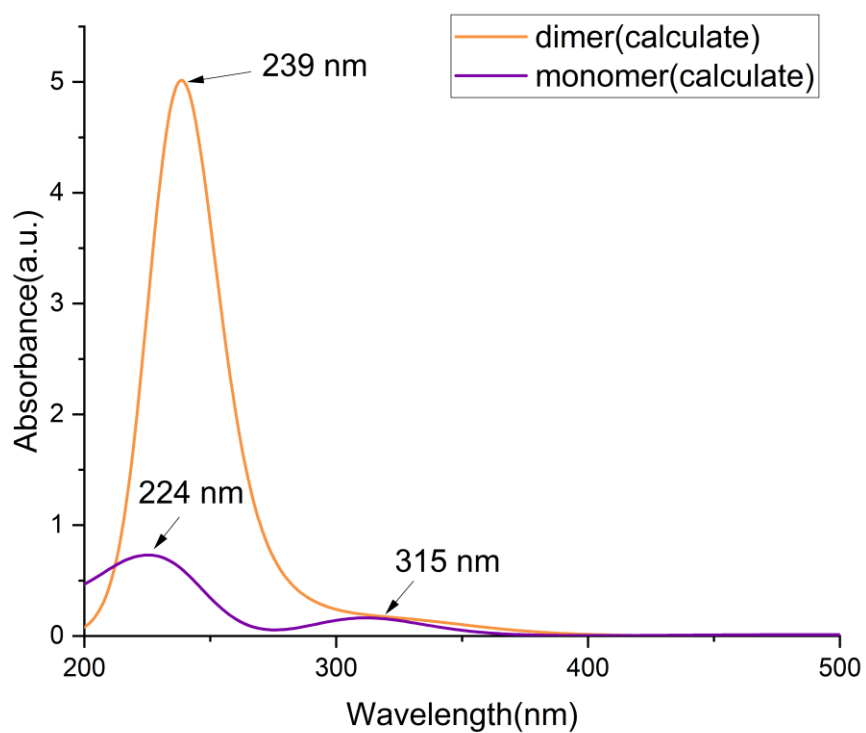
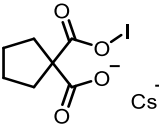
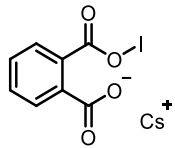
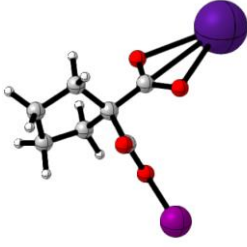
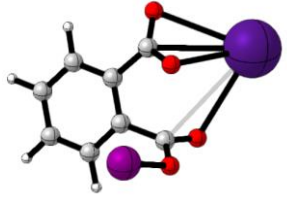
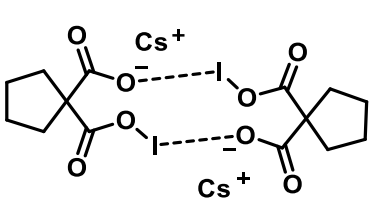
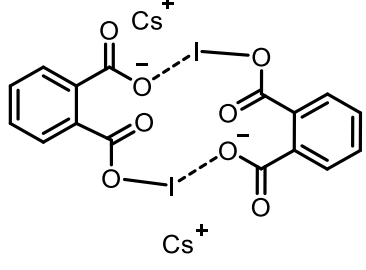
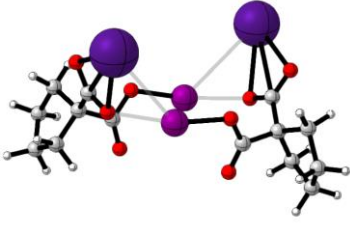
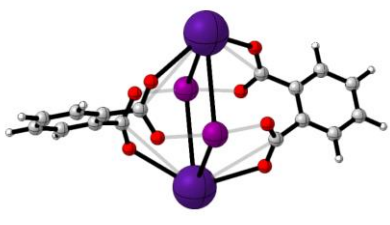


Figure S32. UV/Vis by TDDFT of MPO dimer and monomer about MPO (with TBAB) computed by TDDFT

7.3 Raman spectrum prediction by DFT.

Table S14 Theoretical Raman wavenumbers by B3LYP/Def2-TZVP.

Species		
		
Raman wavenumbers (cm ⁻¹)	191.7	190.0
Species		
		
Raman wavenumbers (cm ⁻¹)	164.6	179.5

We performed DFT calculation (B3LYP/Def2-TZVP) to simulate the Raman spectra of the typical acyl hypoiodite species (**Table S14**). The relevant Raman wavenumbers for monomer acyl hypoiodites are 191.7, 190.0 cm⁻¹, and dimer acyl hypoiodites are 164.6, 179.5 cm⁻¹. Respectively, the dimer structures are very closed to our experimental observation.

7.4 The DFT calculation of potential energy surface

7.4.1. Potential energy surface of the ring-opening halogenation of cycloalkanols

Based on the experimental results and our previous research, we proposed the mechanism as shown in **Figure 5**. The cyclic diacyl peroxides initially reacts with TMAB (simplified model for TBAB) to generate the acyl hypobromite intermediate INT2B, with a free energy barrier of 12.6 kcal/mol. It is noticeable that the acyl hypobromite intermediate INT2B is easily converted into the highly stable dimer **INT2B-d**, with an energy of -24.7 kcal/mol. This is consistent with the occurrence of two identical NMR shifts. This can be also supported by the UV-vis spectrum. The computed UV-vis spectrum of the dimer INT2B-d demonstrates that the strong absorption at 261 nm is in good agreement with the experiment, whereas the monomer **INT2B** exhibits a peak at 206 nm (**Figure S31**). The dimer would then undergo a homolytic cleavage of O-Br bond under the blue LED, producing a radical anion INT4 and the bromine radical. The intermediate INT2B has a lower O-Br bond dissociation enthalpy (BDE) than the comparable acyl hypobromite without COO⁻, suggesting that the COO⁻ is critical for the stability of the radical anion species (**Figure S33**). It is worth noting that the O-Br BDE of the hypobromite generated from the substrate is substantially higher than the **INT2B** (**Figure S38**, a similar instance is found in our earlier study). The novel radical anion **INT4** would then abstract hydrogen from the substrate by homolytic cleavage of O-H bond to generate the oxygen radical and the byproduct TDRA-H. The energy barrier for this step is only 19.3 kcal/mol, which could partially attribute to the concerted proton transfer.

In contrast, the polar pathway starts from the acyl hypobromite to undergo O-H bond cleavage directly, requiring an energy barrier of 43 kcal/mmol (**Figure S34**). Thus, this pathway can be excluded from both experiment and computation.

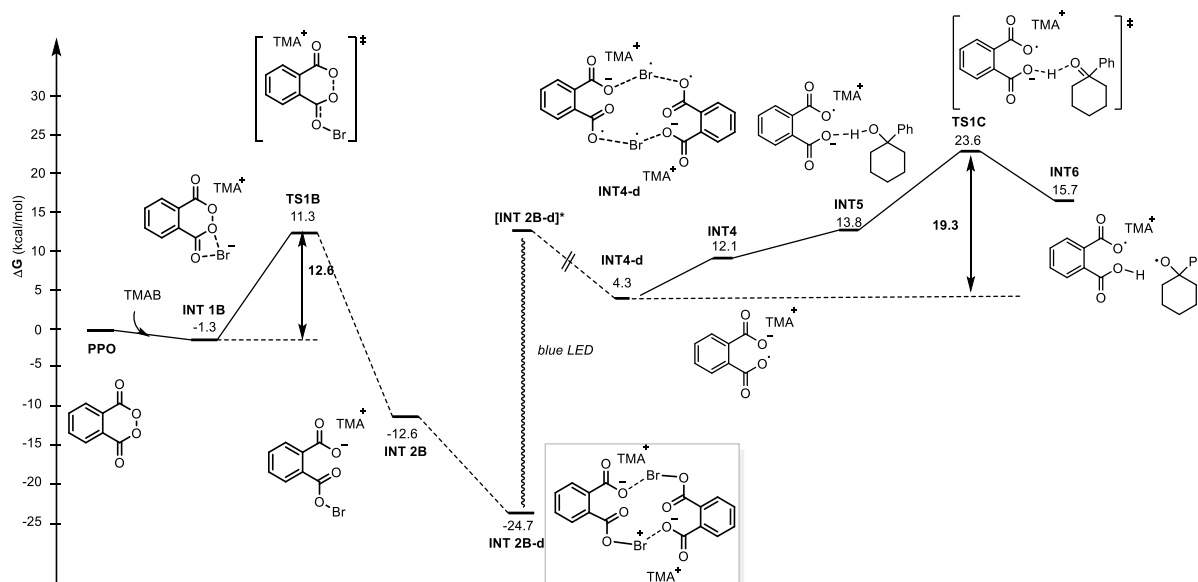


Figure S33. The Gibbs free energy potential surface for the PPO/TMA computed at M052X/6-31G(d)/SMD(1,2-dichloroethane)//B3LYP/6-31+G(d) level of theory.

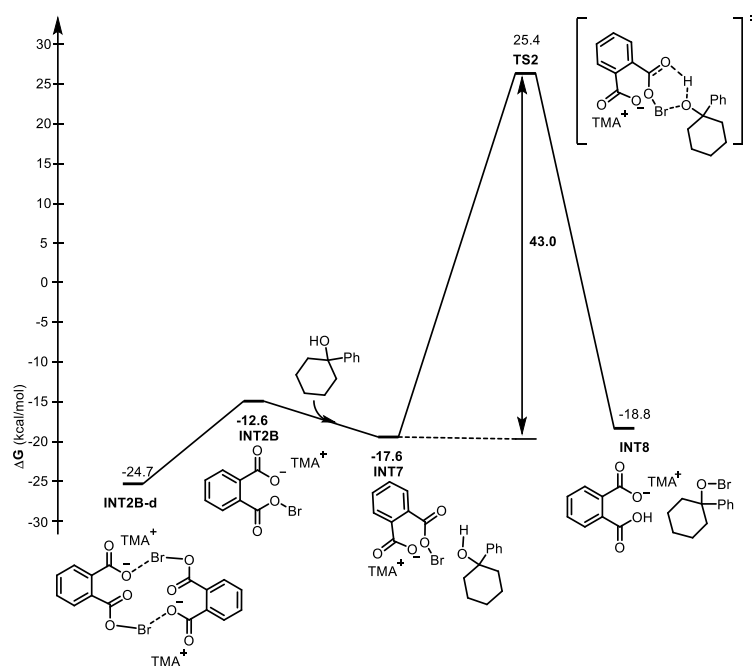


Figure S34. The Gibbs free energy potential surface for the O-Br pathway computed at M052X/6-31G(d)/SMD(1,2-dichloroethane)//B3LYP/6-31+G(d) level of theory.

7.4.2. Potential energy surface of the C(sp³)-H amination of imidates

The half part of the β - and γ -aminations of imidates (the PCET process of NCRs), the activation energy of TS3 and TS4 were calculated to be 11.1 kcal/mol and 10.9 kcal/mol higher than that of INT10 and INT12, respectively (**Figure S35**), therefore the 1,5- or 1,6-HAT is the rate-determining step.

In contrast, the polarity pathway starts from the acyl hypiodite to undergo N-H bond cleavage directly, requiring an energy barrier of 39.8 kcal/mmol (**Figure S36**). Thus, this pathway can be excluded from both experiment and computation.

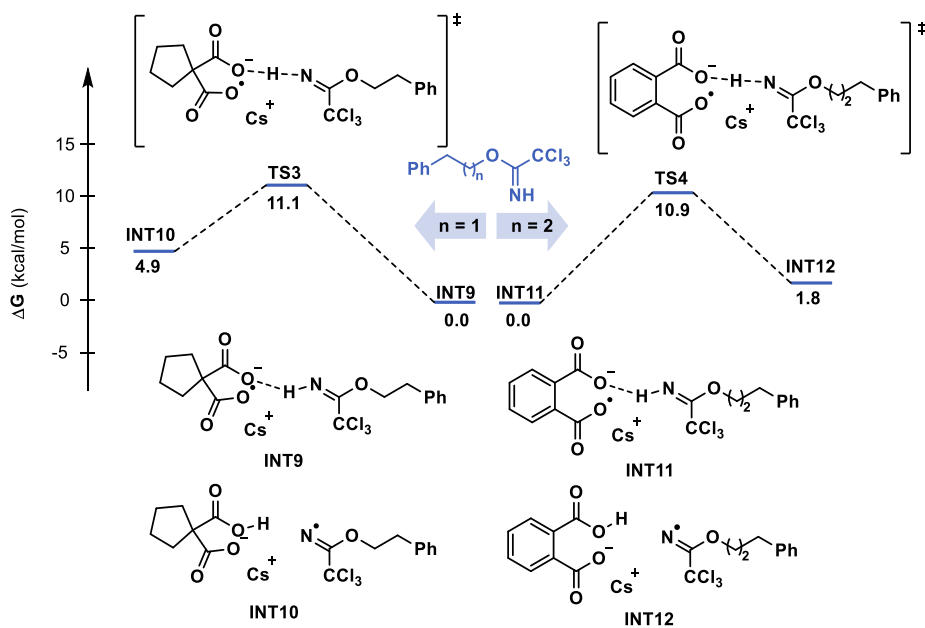


Figure S35. The Gibbs free energy potential surface for the TDRA-induced pathway computed at S63

M052X/6-31G(d)/SMD(MeCN)//B3LYP/6-31+G(d) level of theory.

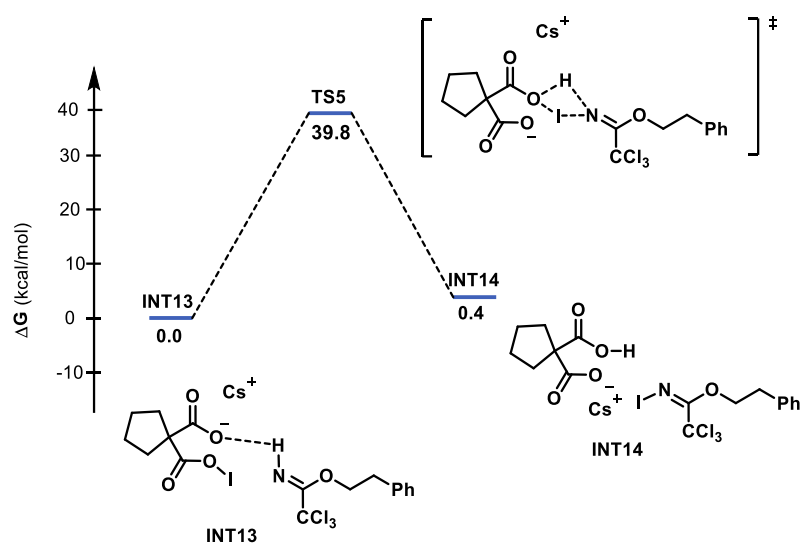
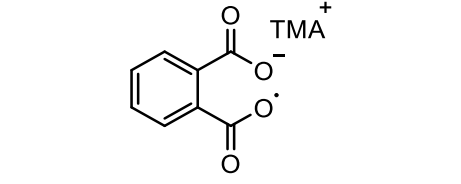
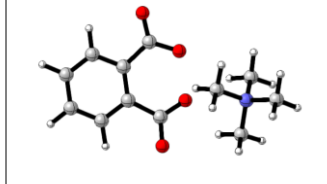
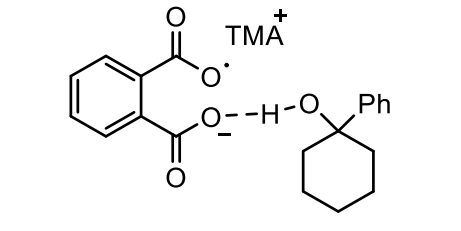
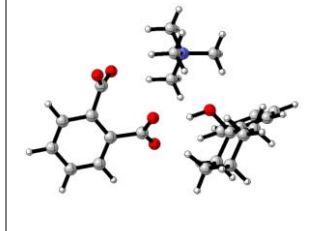
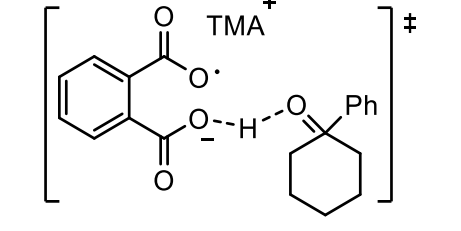
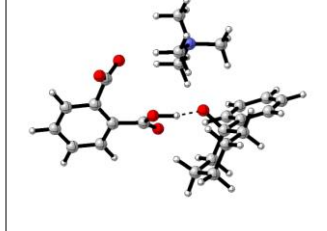
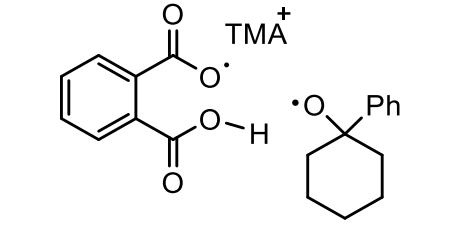
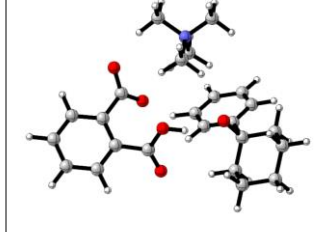


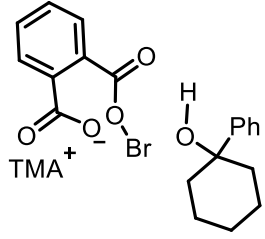
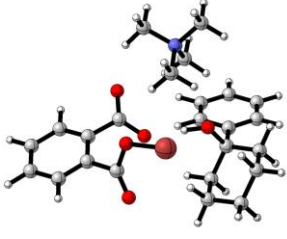
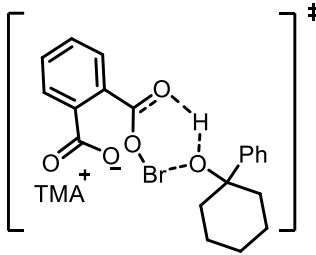
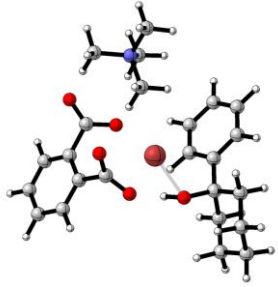
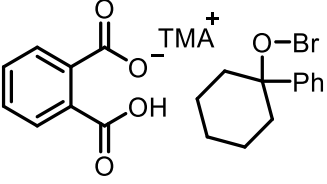
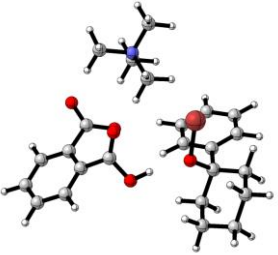
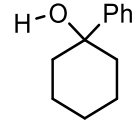
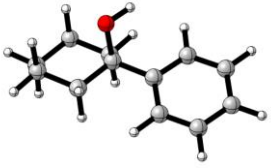
Figure S36. The Gibbs free energy potential surface for the N-I pathway computed at M052X/6-31G(d)/SMD(MeCN)//B3LYP/6-31+G(d) level of theory.

Table S15. Absolute energies (a.u.) calculated at the M052X/6-31G(d)/SMD(1,2-dichloroethane) or M052X/6-31G(d)/SMD(MeCN) level and absolute energies calculated by M052X/6-31G(d)/SMD(1,2-dichloroethane)//B3LYP/6-31+G(d) or M052X/6-31G(d)/SMD(MeCN)//B3LYP/6-31+G(d)

	Species	Optimized Structures	Sum of electronic and thermal Free Energies (a.u.) ^a	Gas-electronic Energies (a.u.) ^b	Solvent-electronic Energies (a.u.) ^c	Solvent-corrected electronic and thermal Free Energies (a.u.) ^d	<S ² >
PPO			-608.032009	-607.995	-608.01	-608.04	/
TMAB			-2785.687738	-2785.72	-2785.76	-2785.72	/
INT1B			-3393.728064	-3393.74	-3393.78	-3393.76	/

TS1B			-3393.71	-3393.75	-3393.7	-3393.74	/
INT2B			-3393.76	-3393.8	-3393.745748	-3393.78	/
INT2B-d			-6787.59	-6787.65	-6787.5	-6787.60	/
INT4-d			-6787.5	-6787.59	-6787.65	-6787.51	/

INT4			-822.36	-822.403	-822.3	-822.36	0.761061
INT5			-1364.46	-1364.5	-1364.29	-1364.33	0.758474
TS1C			-1364.44	-1364.48	-1364.28	-1364.31	0.75744
INT6			-1364.46	-1364.51	-1364.28	-1364.33	0.756033

INT7			-3935.72	-3935.86	-3935.91	-3935.76	/
TS2			-3935.64	-3935.74	-3935.8	-3935.69	/
INT8			-3935.72	-3935.86	-3935.91	-3935.76	/
1-phenyl cyclohexanol			-541.958	-542.068	-542.085	-541.97	/

INT9			-2490.11	-2490	-2490.05	-2490.15	0.755206
INT10			-2490.1	-2490.01	-2490.06	-2490.14	0.758609
TS3			-2490.08	-2489.97	-2490.03	-2490.13	0.757646
INT11			-2565.13	-2564.99	-2565.04	-2565.18	0.757755
INT12			-2565.12	-2565.01	-2565.07	-2565.17	0.757748

TS4			-2565.11	-2564.97	-2565.03	-2565.16	0.757514
INT13			-2501.55	-2501.43	-2501.48	-2501.60	/
INT14			-2501.55	-2501.43	-2501.48	-2501.59	/
TS5			-2501.47	-2501.34	-2501.4	-2501.53	/

^aAbsolute values of Gibbs free energy (G) by B3LYP/6-31+G(d). ^bAbsolute values of electronic energies (EE) by M052X/6-31G(d). ^c Absolute values of electronic energies (EE) by M052X/6-31G(d)/SMD(1,2-dichloroethane) or M052X/6-31G(d)/SMD(MeCN). ^dAbsolute values of Gibbs free energy by M052X/6-

31G(d)/SMD(1,2-dichloroethane)//B3LYP/6-31+G(d) or M052X/6-31G(d)/SMD(MeCN)//B3LYP/6-31+G(d). Subtracting the value in this column 5 from the value in column 6 produces the solvation free energy. At 298.15K, the free energy change corresponding to the change in gas concentration from 1atm to 1M is 1.89kcal/mol. Addition of the value in column 4 to the solvation free energy produces the solvent-corrected Gibbs free energy. The given energy values in a.u. can be converted to kcal/mol via the multiplication factor of 627.5095.

7.5 The details of the BDEs

Homolytic bond dissociation enthalpies (BDE) for a number of molecules by using B3LYP-D3/6-311+G(d,p)//B3LYP-D3/6-31+G(d)//SDD(Cs and I).

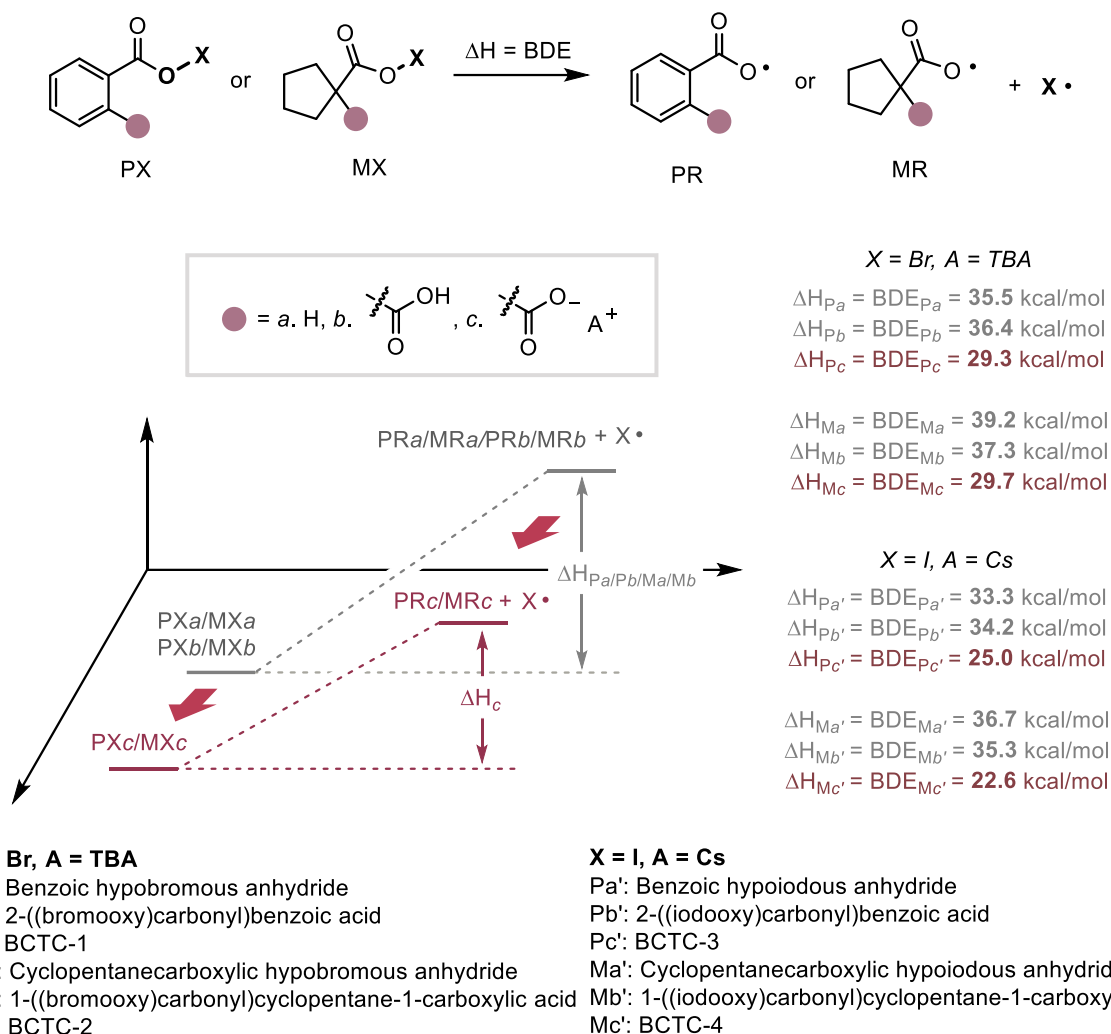


Figure S37. The BDEs of different radicals to explain the differences in stability

Stability of Radicals and O/N-Halogenated Compounds

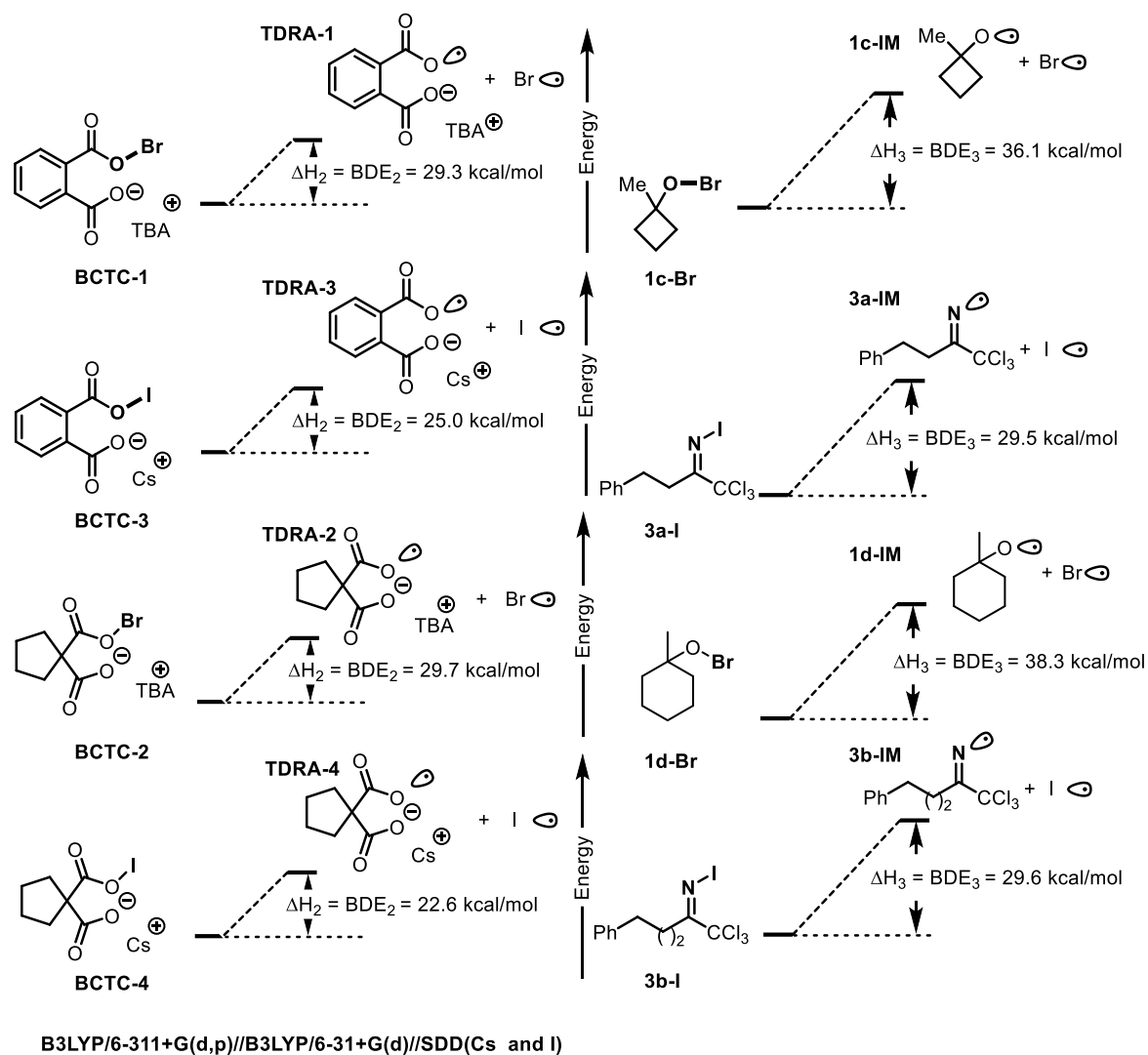


Figure S38. The stability of radicals and O/N-Halogenated compounds

7.6 SOMO-HOMO inversion

Ordering and occupation of molecular orbitals (e.g. SOMO and HOMO) of TDRA were evaluated by density functional theory with triple ζ basis set (Def2-TZVP) following geometry optimization at the B3LYP/6-31+G(d).

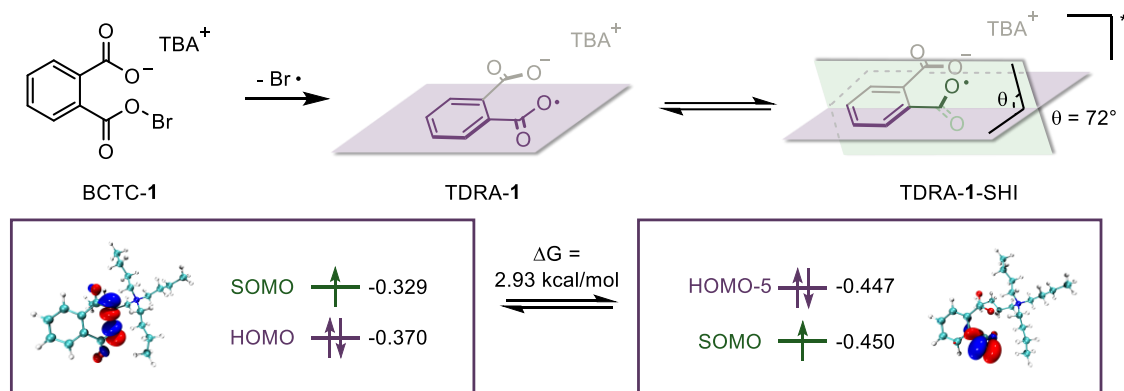


Figure S39. The SOMO-HOMO inversion of TDRA calculated by M062X/Def2-TZVP.

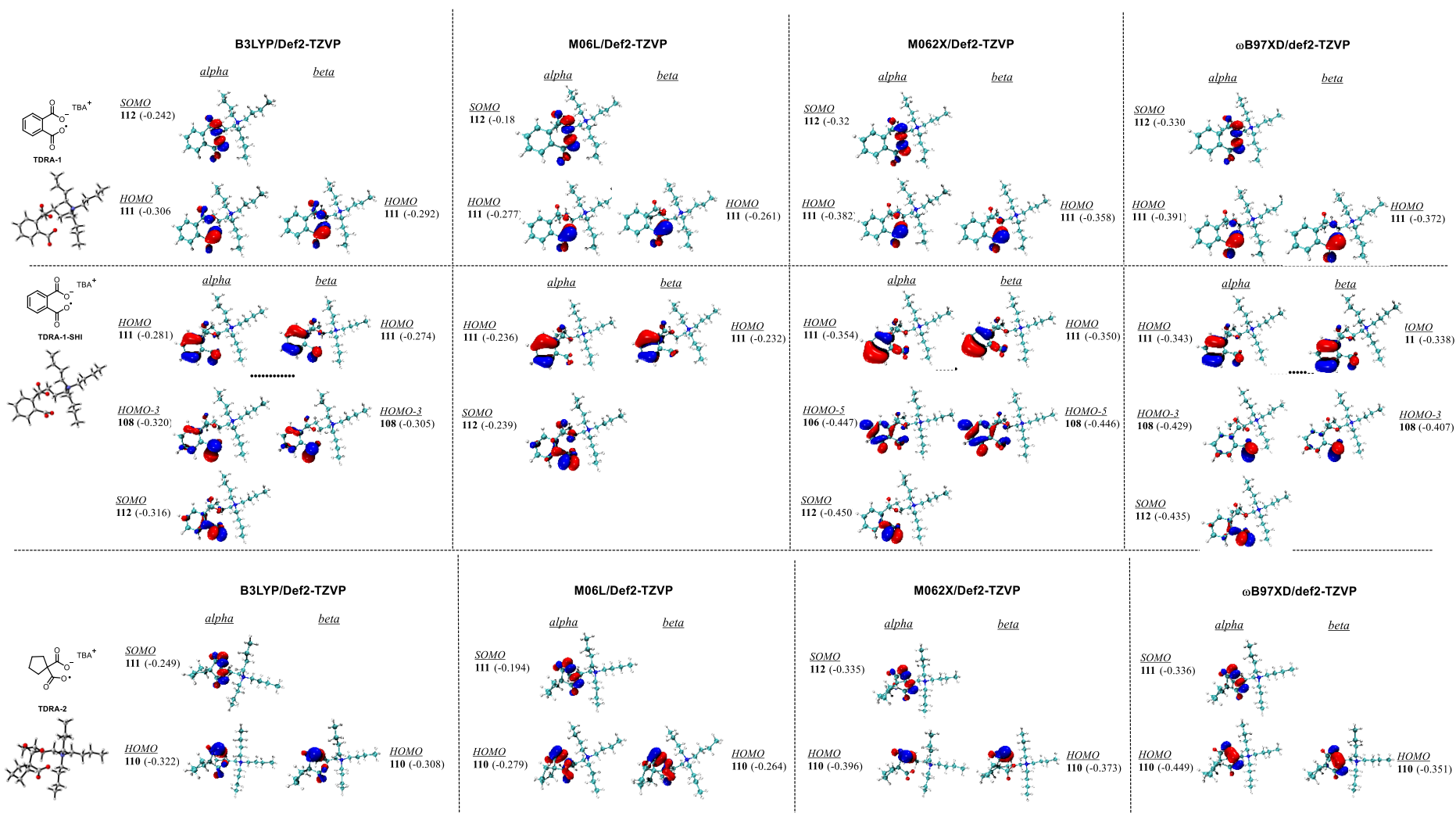


Figure S40. The molecular orbitals of TDRA calculated by density functional theory with triple ζ basis set (Def2-TZVP). The numbers are the alpha and beta orbital energies

8. Properties of the TDRA

8.1 Electrophilicity and Nucleophilicity Index

Commonly N refers to the number of electrons carried by a chemical system at its most stable status. Geometry optimized for N electrons state is employed for all calculations.

$$\text{Electrophilicity index}^{58} (\omega): \omega = \frac{\mu^2}{2\eta}$$

Nucleophilicity index⁵⁹ (N_{Nu}): $E_{HOMO}(Nu) - E_{HOMO}(TCE)$ where Nu denotes nucleophile, TCE denotes tetracyanoethylene. HOMO energy of TCE were calculated using B3LYP-D3/6-311+G(d,p) method

$$\text{Condensed local electrophilicity index}^{60} (\omega_{rc}^+): \omega_{rc}^+ = \omega f_{rc}^+$$

$$\text{Condensed local electrophilicity index}^{61} (N_{rc}): N_{rc} = N_{Nu} f_{rc}^-$$

The electrophilicity index ω_{cubic} introduced in J. Phys. Chem. A, 124, 2090 (2020) is somewhat special, it is the only quantity that also relies on $N-2$ electron states. Its definition is

$$\omega_{cubic} = \omega \left(1 + \frac{\mu}{3\eta^2} \gamma \right)$$

The definition of condensed Fukui function for an atom, say A , can be written as




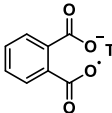
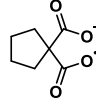
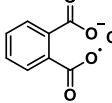
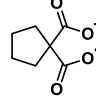

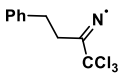
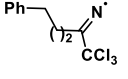



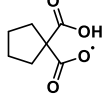
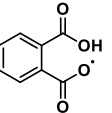


$$f_A^+ = P_{N+1}^A - P_N^A$$

Where P^A is the electron population number of atom A

Geometries of all species were fully optimized using B3LYP functional with dispersion correction (GD3) and 6-31+G(d) basis set. More accurate electronic energies were calculated using B3LYP/6-311+G(d,p) method

Table S16. Electrophilicity and Nucleophilicity Index of some radicals

○ Electrophilicity index (ω); Cubic electrophilicity index (ω_{cubic}); Nucleophilicity index (N); Condensed local electrophilicity index (ω_{rc}^+); Condensed local cubic electrophilicity index ($\omega_{\text{cubic(rc)}}$); Condensed local nucleophilicity index (N_{rc}) --- All values are in eV. (B3LYP/6-311+g(d,p))

	ω	ω_{cubic}	N	ω_{rc}^+	$\omega_{\text{cubic(rc)}}$	N_{rc}	
Strong Nucleophilic		0.600	0.402	4.968	0.126	0.084	1.324
		0.822	0.889	4.278	-0.001	-0.001	1.252
		0.846	0.993	3.977	-0.006	-0.005	0.669
weak Nucleophilic		1.579	1.716	3.199	0.291	0.317	0.390
		1.698	1.828	3.378	0.358	0.385	0.454
		1.718	1.847	3.117	0.286	0.307	0.418
		1.765	1.896	3.321	0.326	0.351	0.436
Weak to moderate Electrophilic		2.056	2.182	2.681	0.781	0.829	0.209
		2.121	2.277	2.275	0.726	0.780	0.367
		2.117	2.262	2.518	0.725	0.775	0.390
		2.231	2.212	2.851	0.490	0.486	0.512
		2.807	2.919	0.927	0.953	0.991	0.295
Strong Electrophilic		2.809	2.932	0.531	2/070	2.161	0.423
		3.053	3.080	1.216	0.968	0.976	0.175
		3.114	3.092	1.442	0.903	0.897	0.160
		3.116	3.113	1.665	1.202	1.200	0.121
		3.705	3.762	0.970	3.703	3.759	0.970

8.2 Quantitative analysis of molecular surface

8.2.1. Electrostatic potential on vdW surface (EPS).

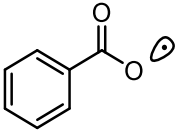
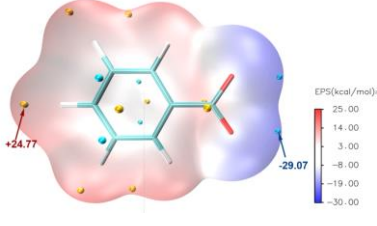
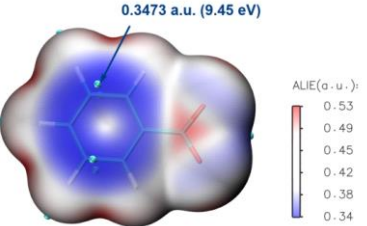
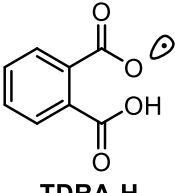
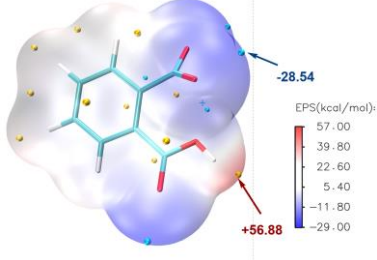
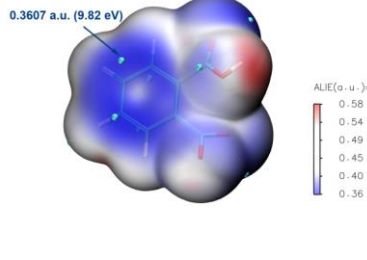
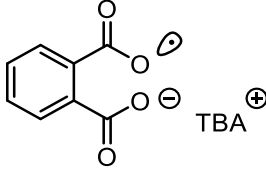
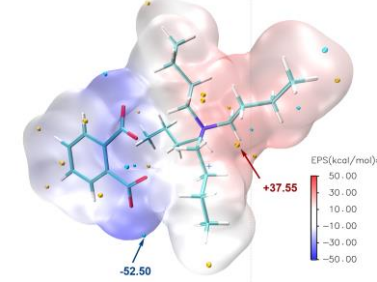
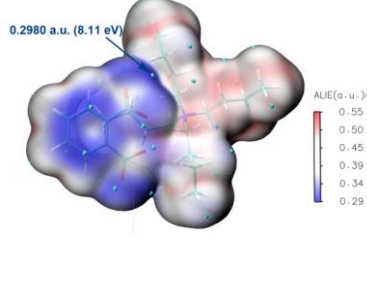
Molecular electrostatic potential⁶²⁻⁶⁴ (EPS), $V(r)$, has been widely used for prediction of nucleophilic and electrophilic sites, as well as molecular recognition mode for a long time, the theoretical basis is that molecules always tend to approach each other in a complementary manner of EPS. Geometries of all species were fully optimized using B3LYP-GD3 and 6-31+G(d) basis set. More accurate electronic energies were calculated using B3LYP/6-311+G(d,p) method

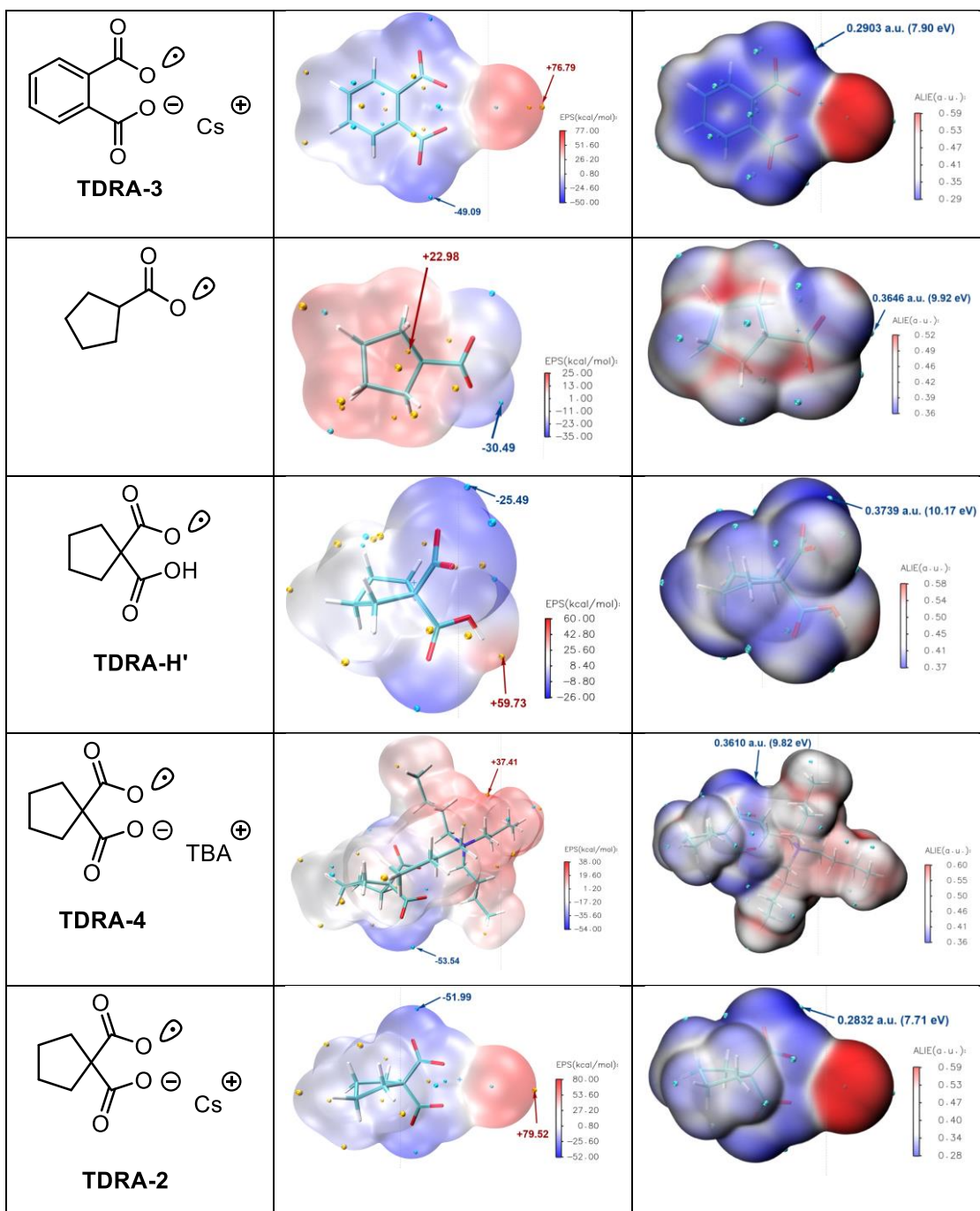
8.2.2. Average local ionization energy (ALIE).

Average local ionization energy^{65,66}, I^- , has the most important use maybe the was used to predict the ion of reactivity according to function value on vdW surface, I^-_S . Lower value of I^-_S indicates that the electron at r is more weakly bounded, therefore r is more likely r is the site of electrophilic or radical attack. Geometries of all species were fully optimized using B3LYP functional with dispersion correction and 6-31+G(d) basis set. More accurate electronic energies were calculated using B3LYP/6-311+G(d,p) method

Using Multiwfn⁶⁷ combined with VMD⁶⁸ analysis and drawing of molecular surface.

Table S17. EPS and ALIE of different species.

Species	EPS ^a	ALIE ^b
		
 TDRA-H		
 TDRA-1		

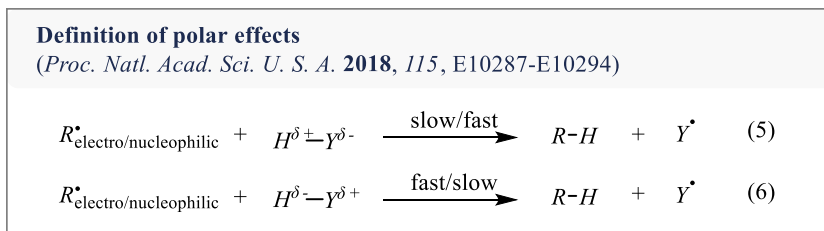
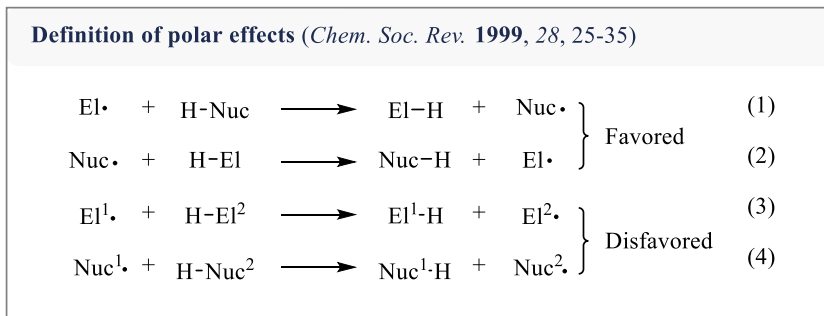


a. Electrostatic potential (EPS) mapped van der Waals surface ($\rho = 0.001$ a.u.). The red color represents the positive ESP. Minima and maxima of ESP on the surface are drawn as cyan and orange spheres, respectively. **b.** Average local ionization energy. The blue color represents lower \bar{I}_S .

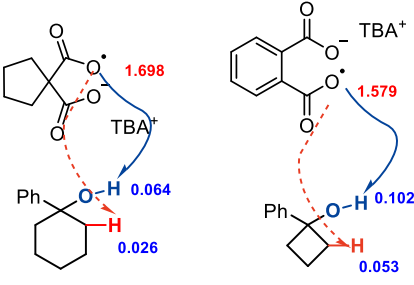
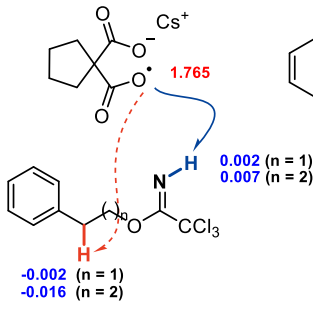
9. Computational studies of PCET

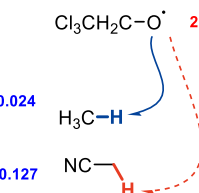
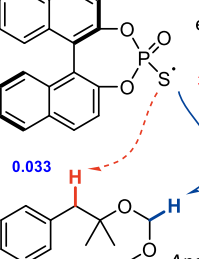
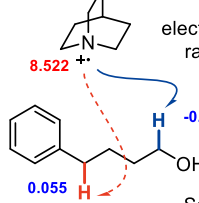
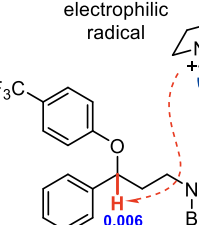
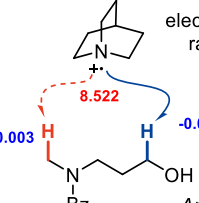
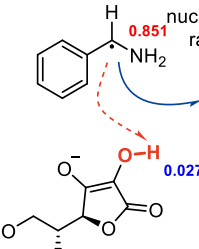
9.1 Polarity matching

Some typical reports about polarity-matched HAT were listed in **Figure S41**. The blue arrows represent the experimentally successful abstraction, while the red arrows mean the abstraction pathway not detected by authors' experiment. In order to better understand the polarity matching in specific examples⁶⁹⁻⁷⁹, we conducted density functional theory (DFT) calculations for corresponding structures. Specifically, we determined dual descriptor Fukui function values (blue numbers) for hydrogen atom and Electrophilicity index (red numbers) of for radicals. The more positive condensed dual descriptor (CDD) values are, the more electrophilic the corresponding site hydrogen is. In addition, the higher the values of Electrophilicity index are, the more electrophilic the radicals are. Evaluated the matching degree by these rules, some consistent examples demonstrate that is helpful to use theoretical calculation to predict polarity matching. Some consistent examples show that using theoretical calculations to predict polarity matching is beneficial.



- The **PME** approach lacks any quantitative prediction ability.
- **PME** rules can be difficult to apply to a broad spectrum of **PCET agents**, including transition-metal systems in which donors and acceptors for electron vs. proton may reside on different sites and the distinction between electrophilic and nucleophilic oxidants can be subtle or ambiguous.

The reported polar effects in HAA and the calculated Electrophilicity index of radicals, the calculated Condensed dual descriptor of hydrogen atom	Descriptions in the literature (based on experiences)	Conclusions based on calculated data
		Polarity-matched
<p>distonic radical anion from MPO</p> 		Polarity-matched

The reported polar effects in HAA and the calculated Electrophilicity index of radicals, the calculated Condensed dual descriptor of hydrogen atom	Descriptions in the literature (based on experiences)	Conclusions based on calculated data
 <p>Cl₃CH₂C-O• 2.323 electrophilic radical 0.024 H₃C-H 0.127 NC-H <i>Science</i>, 2018, 361, 668</p>	Polarity-matched	Polarity-matched
 <p>electrophilic radical 3.402 0.033 H 0.002 H neutral C-H: ~90 kcal/mol hydric C-H: ~93 kcal/mol <i>Angew.Chem.Int. Ed.</i> 2018, 57,10357</p>	Polarity-matched	Polarity-matched
 <p>electrophilic radical 8.522 0.055 H -0.017 H Strong C-H weaker C-H <i>Science</i>, 2015, 349, 1532</p>	Polarity-matched	Polarity-matched
 <p>electrophilic radical 8.522 0.006 H -0.015 H neutral C-H: ~86 kcal/mol hydric C-H: ~92 kcal/mol <i>Nature</i> 2017, 547, 79</p>	Polarity-matched	Polarity-matched
 <p>electrophilic radical 8.522 0.003 H -0.023 H <i>Angew.Chem. Int.Ed.</i> 2018, 57, 5369</p>	Polarity-matched	Polarity-matched
 <p>nucleophilic radical 0.851 0.064 H-S 0.027 O-H O-H: 72.3 kcal/mol S-H: 87.4 kcal/mol <i>Angew. Chem. Int. Ed.</i> 2018, 57, 2469</p>	Polarity-matched	Polarity-matched

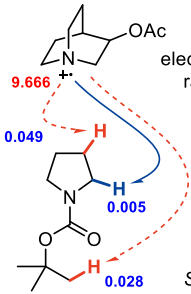
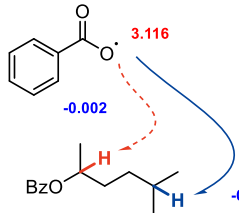
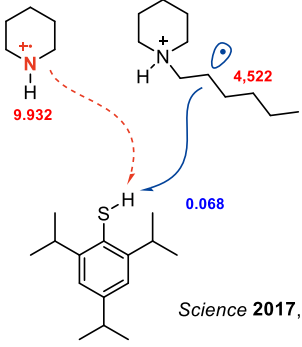
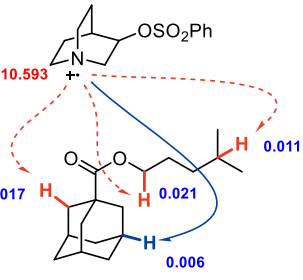
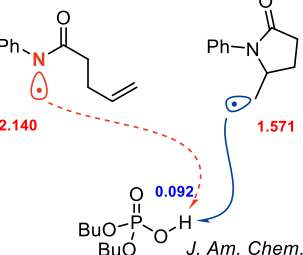
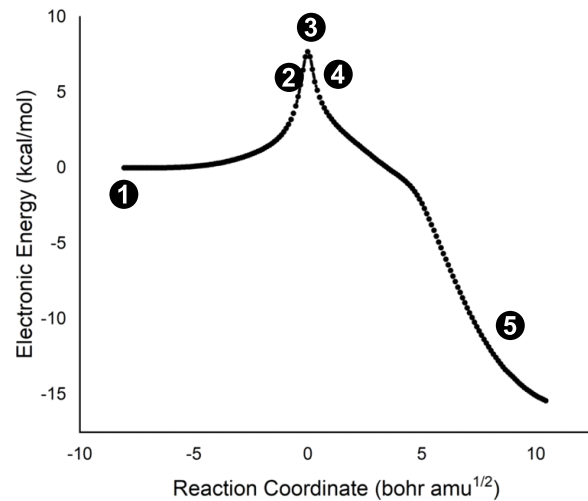
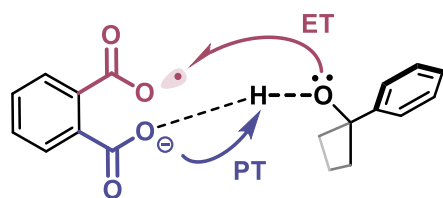
The reported polar effects in HAA and the calculated Electrophilicity index of radicals, the calculated Condensed dual descriptor of hydrogen atom	Descriptions in the literature (based on experiences)	Conclusions based on calculated data
 <p>electrophilic radical</p> <p>9.666</p> <p>0.049</p> <p>0.005</p> <p>0.028</p> <p><i>Science</i> 2016, 352, 1304-1308</p>	Polarity-matched	Polarity-matched
 <p>3.116</p> <p>-0.002</p> <p>-0.005</p> <p><i>J. Am. Chem. Soc.</i> 2016, 138, 16200-16203</p>	Polarity-matched	Polarity-matched
 <p>9.932</p> <p>4.522</p> <p>0.068</p> <p><i>Science</i> 2017, 355, 727-730</p>	Polarity-matched	Polarity-matched
 <p>10.593</p> <p>0.011</p> <p>0.021</p> <p>0.006</p> <p>Strong C-H weaker C-H</p> <p><i>ACS Catal.</i> 2019, 9, 5708-5715</p>	Polarity-matched	Polarity-matched
 <p>2.140</p> <p>1.571</p> <p>0.092</p> <p><i>J. Am. Chem. Soc.</i> 2015, 137, 13492-13495</p>	Polarity-matched	Polarity-matched

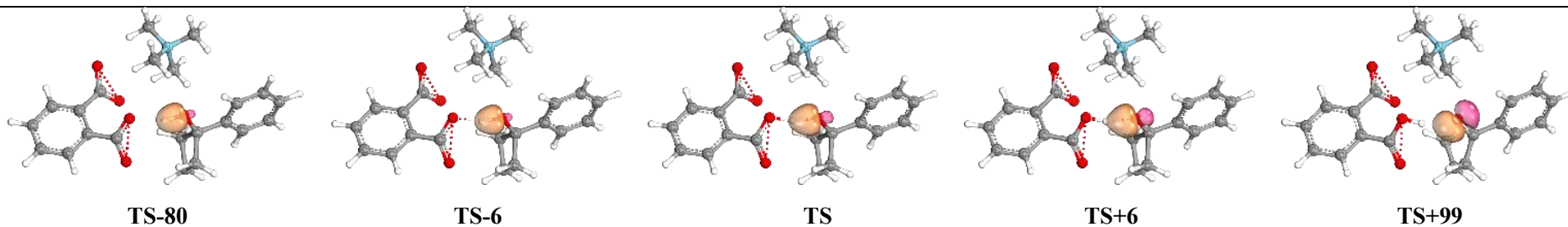
Figure S41. Examples of polarity matching

9.2 IBO analyses

As discussed in the text, IBO analysis allows us to analyze the electron transformation in electronic structure by following changes in the localized IBO for the α and β spin manifolds separately in open-shell system, providing an intuitive picture of the making events throughout a chemical transformation along an intrinsic reaction coordinate (IRC)⁸⁰. Notable, this approach is instrumental in dissecting the subtleties between HAT and PCET in the specific context of HAA reactions. Evolution of the IBOs along the intrinsic reaction coordinate (IRC) representing mainly E–H (E=O, N) bonds have been monitored for all **TDRAs** and are shown in **Figures S42-S46**, which complements those shown in the text. Points on the IRC are referenced to the TS geometry such that a point “TS-80” represents a geometry, 80-point away from the TS (in the reverse direction) along the H-coordinate. Similarly, the point “TS+6” represents a geometry 6-point past the TS (in the forward direction).



four-membered ring cycloalkanol: O-H α -IBO



four-membered ring cycloalkanol: O-H β -IBO

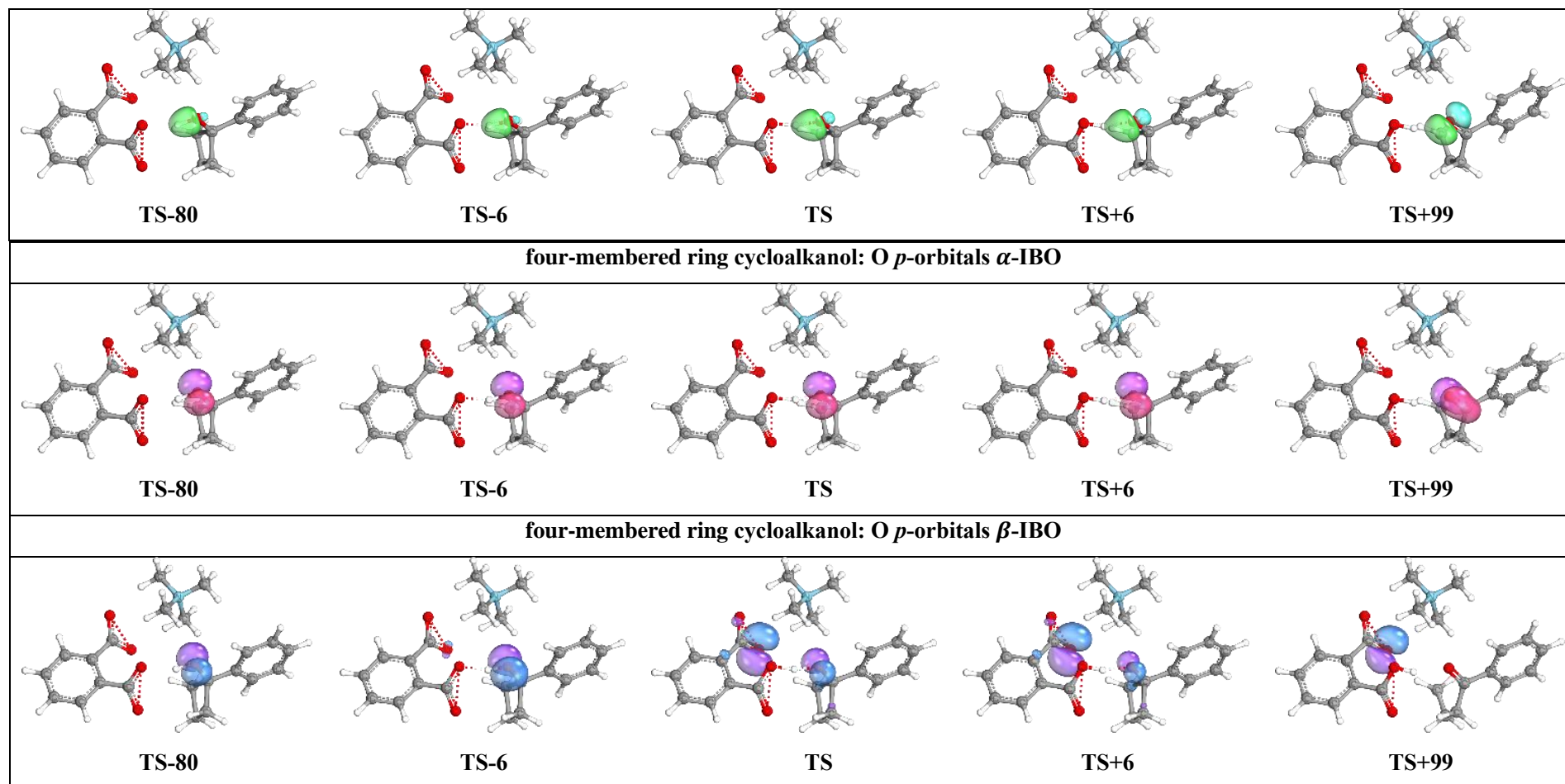
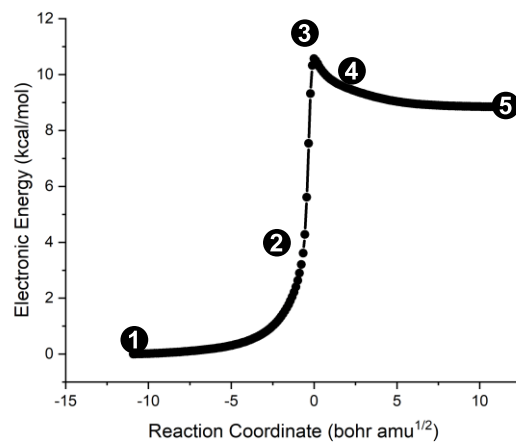
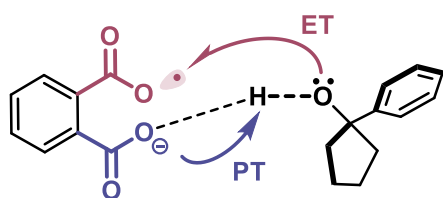
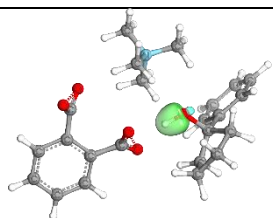


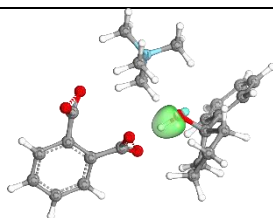
Figure S42. IBOs Figure IBOs relevant for PCET from PPO using cycloalkbutanol. (a) α - and β -IBOs of the O–H bond are shown in orange/pink and green/blue, colors respectively. (b) relevant for PCET from PPO using cycloalkanol α - and β -IBOs of the O p -orbitals are shown in pink/red and purple/blue colors respectively



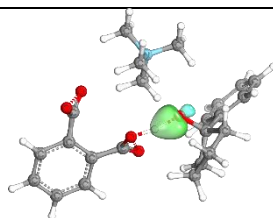
five-membered ring cycloalkanol: O-H α -IBO



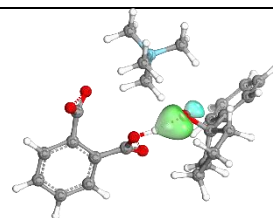
TS-100



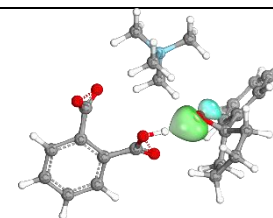
TS-10



TS

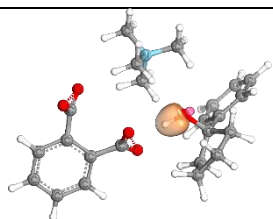


TS+10

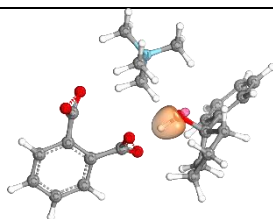


TS+100

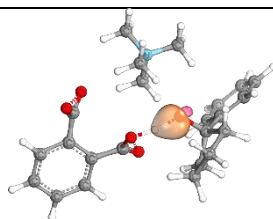
five-membered ring cycloalkanol: O-H β -IBO



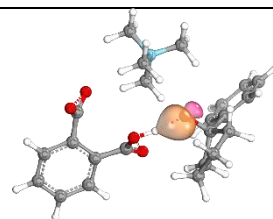
TS-100



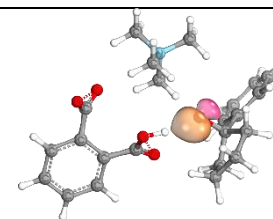
TS-10



TS



TS+10



TS+100

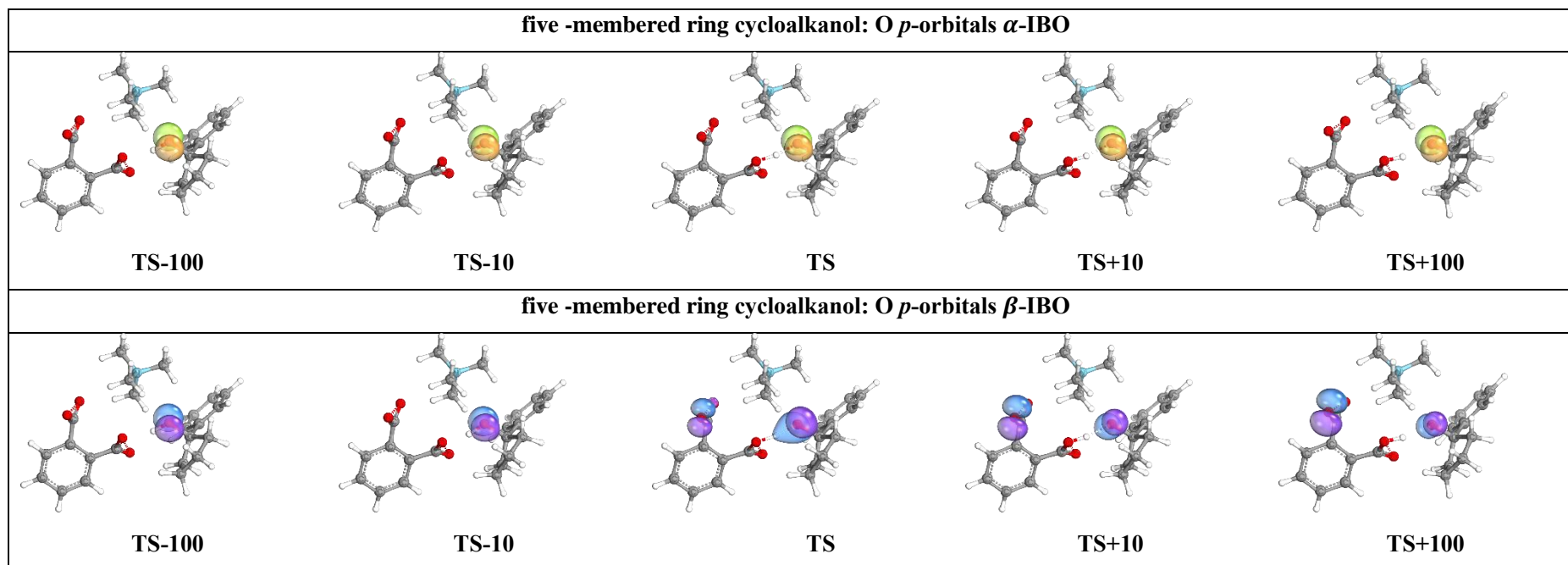
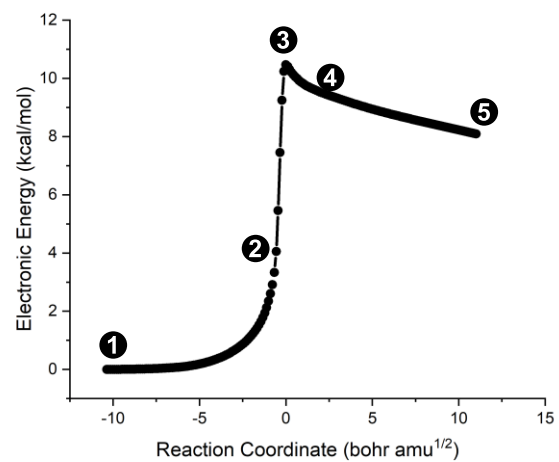
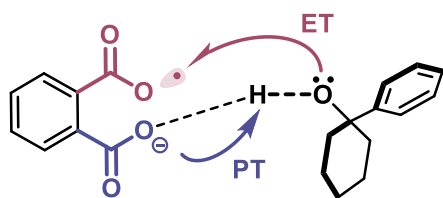
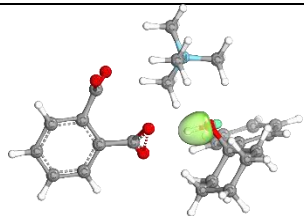


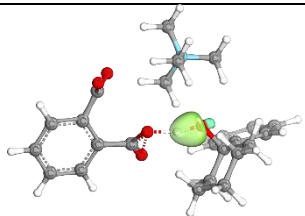
Figure S43. IBOs relevant for PCET from PPO using cyclopentanol. (a) α - and β -IBOs of the O–H bond are shown in green/blue and orange/pink, respectively. (b) α - and β -IBOs of the O *p*-orbitals are shown in orange/green and purple/blue, respectively.



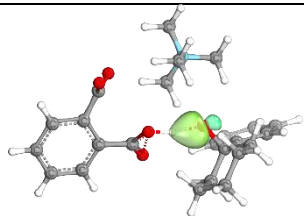
six-membered ring cycloalkanol: O-H α -IBO



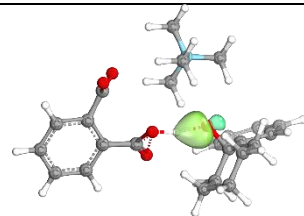
TS-96



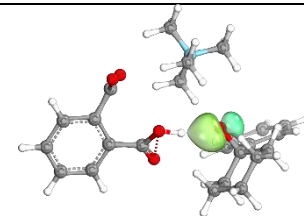
TS-5



TS

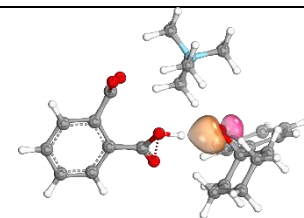
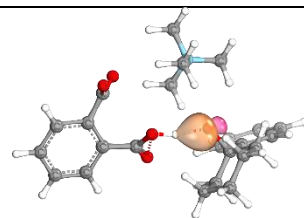
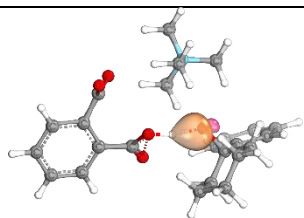
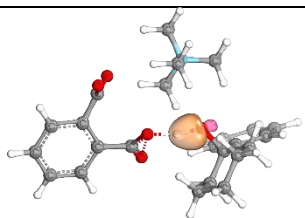
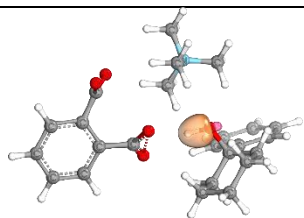


TS+5



TS+96

six -membered ring cycloalkanol: O-H β -IBO



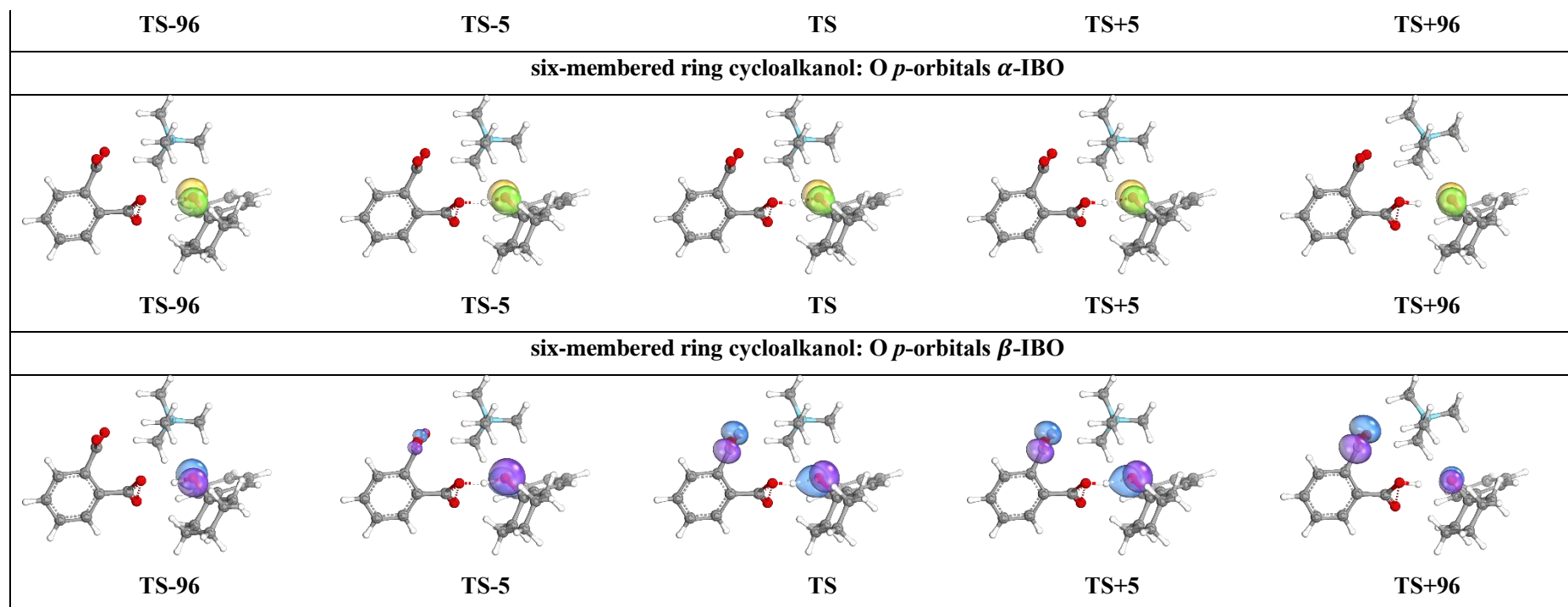


Figure S44. IBOs relevant for PCET from PPO using cyclohexanol. (a) α - and β -IBOs of the O–H bond are shown in green/blue and orange/pink, respectively. (b) α - and β -IBOs of the O *p*-orbitals are shown in orange/green and purple/blue, respectively

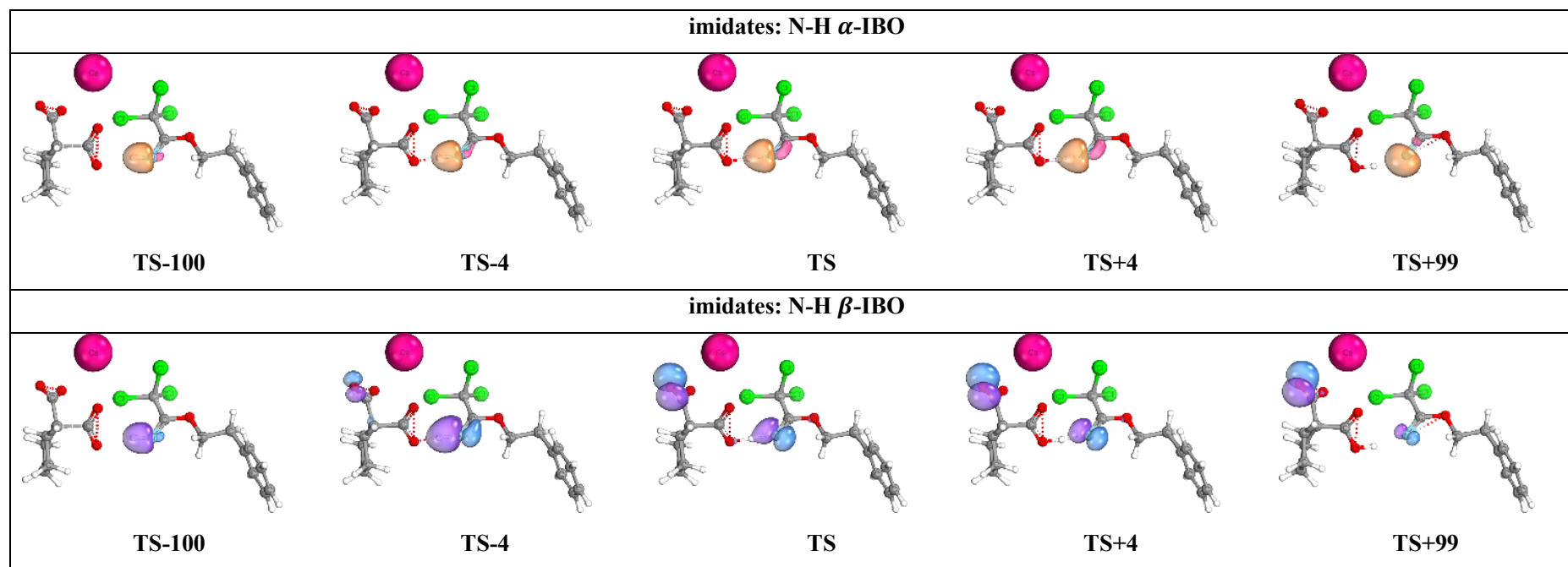
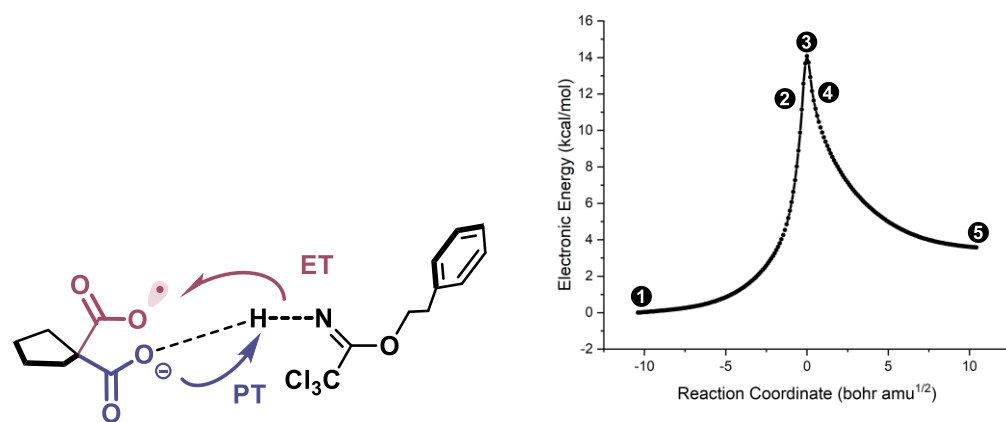


Figure S45. IBOs relevant for PCET from MPO using imidates α - and β -IBOs of the N-H bond are shown in purple/blue and orange/pink colors respectively

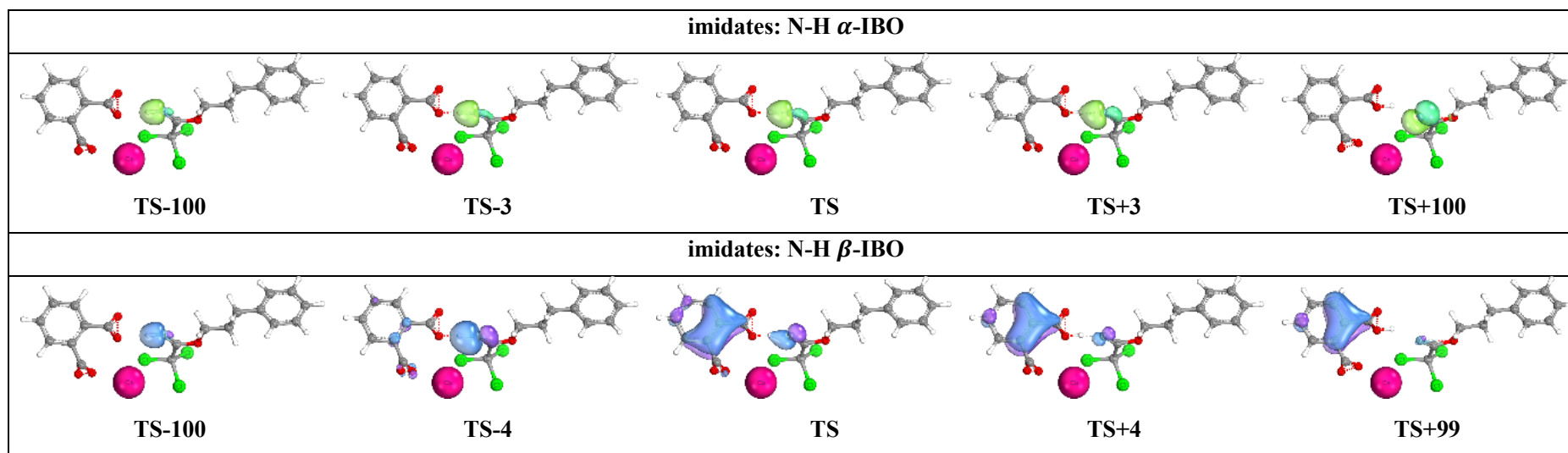
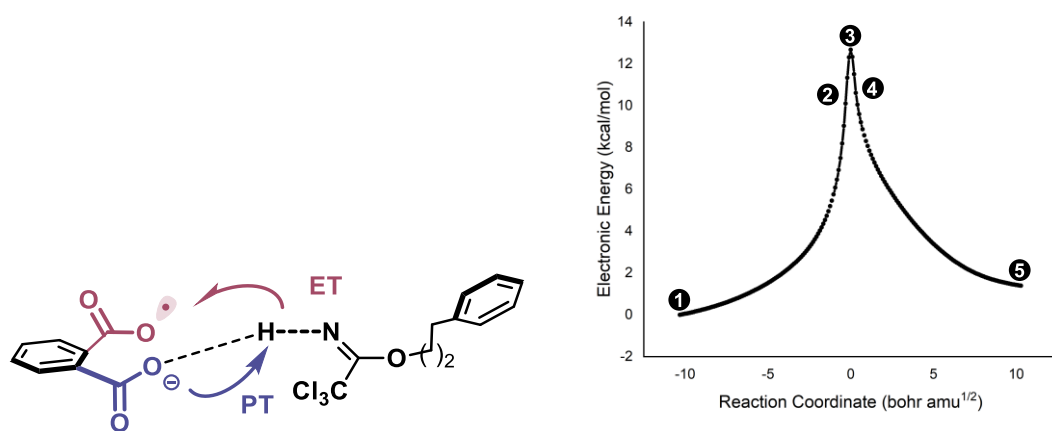


Figure S46. IBOs relevant for PCET from PPO using imidates α - and β -IBOs of the N-H bond are shown in purple/blue and orange/pink colors respectively

9.3 Spin Population Analyses

The changes in the spin densities of the transition states involving proton-coupled proton transfer in the reaction. Points on the IRC are referenced to the TS geometry such that a point “TS-80” represents a geometry, 80-point away from the TS (in the reverse direction) along the H-coordinate. Similarly, the point “TS+6” represents a geometry 6-point past the TS (in the forward direction).

Using Multiwfn⁶⁷ combined with VMD⁶⁸ analysis and drawing of spin populations.

9.3.1 TDRA-1-induced ring-opening bromination of four-membered cycloalkanol.

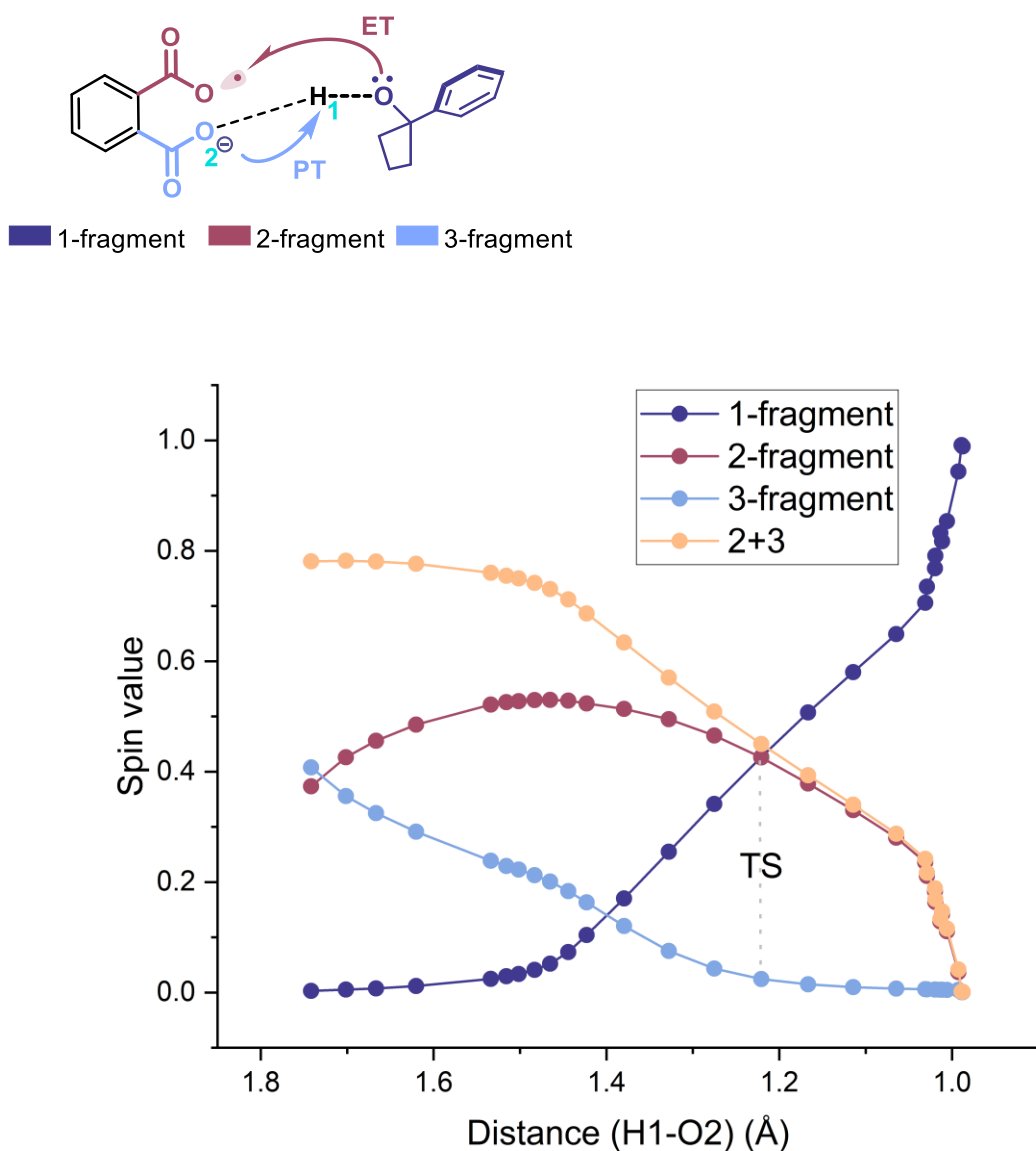


Figure S47. Selected IRC coordinates structure of the open-shell singlet transition state TS to show the change in the spin value of the 1, 2 and 3 fragments

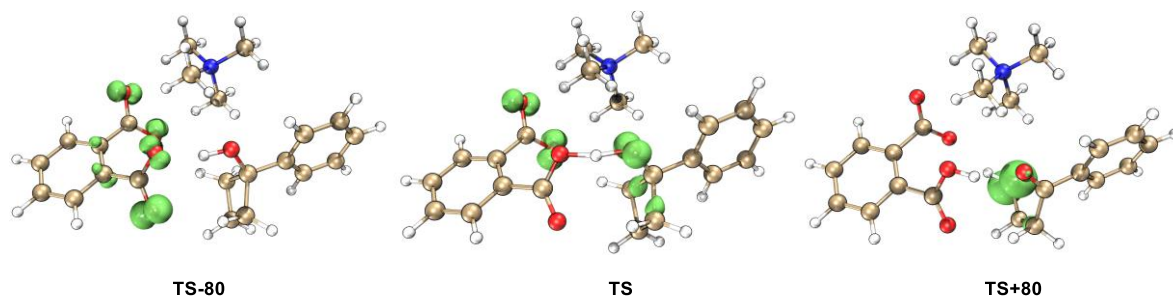


Figure S48. Spin value analysis pictures of open-shell singlet transition states TS, TS-80 and TS+80.
(green, single electron distribution)

9,3,2. TDRA-1-induced ring-opening bromination of five-membered cycloalkanol.

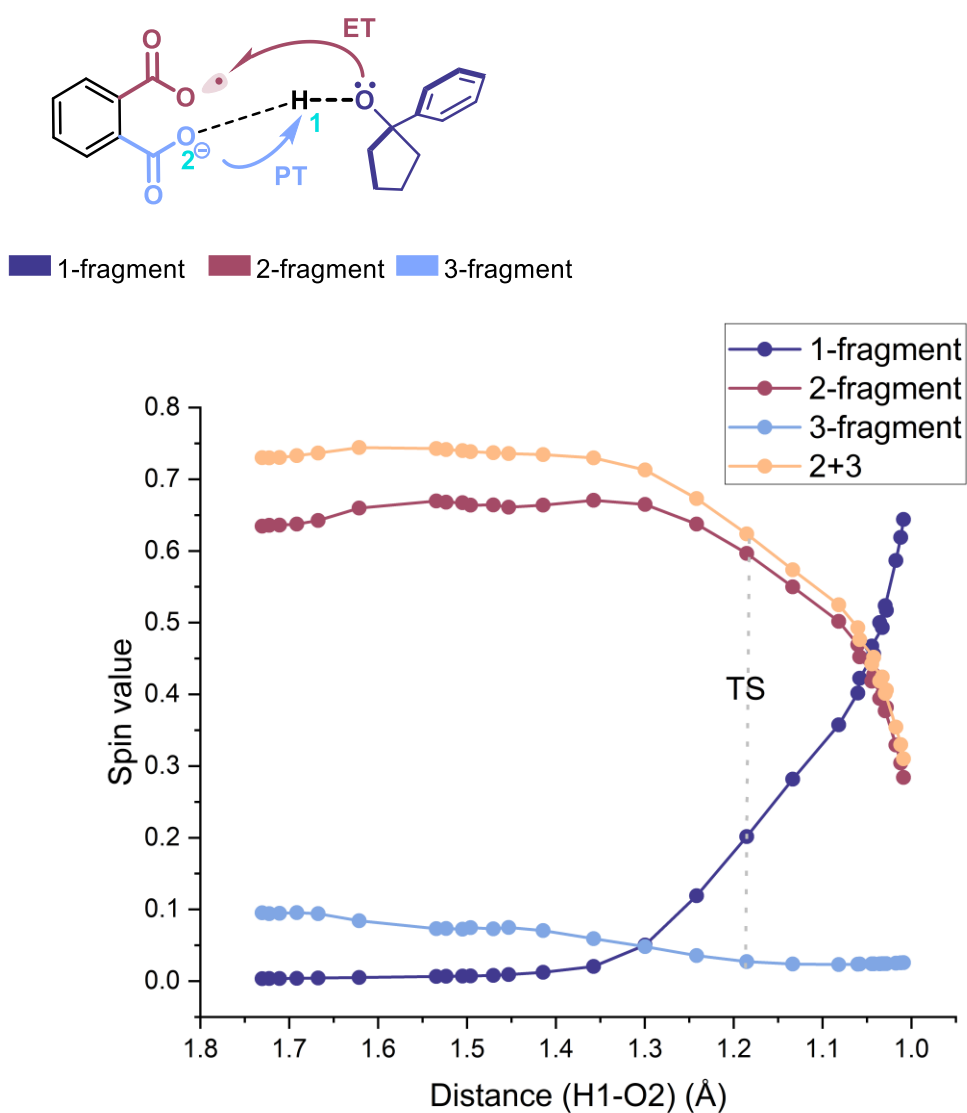


Figure S49. Selected IRC coordinates structure of the open-shell singlet transition state TS to show the change in the spin value of the 1, 2 and 3 fragments

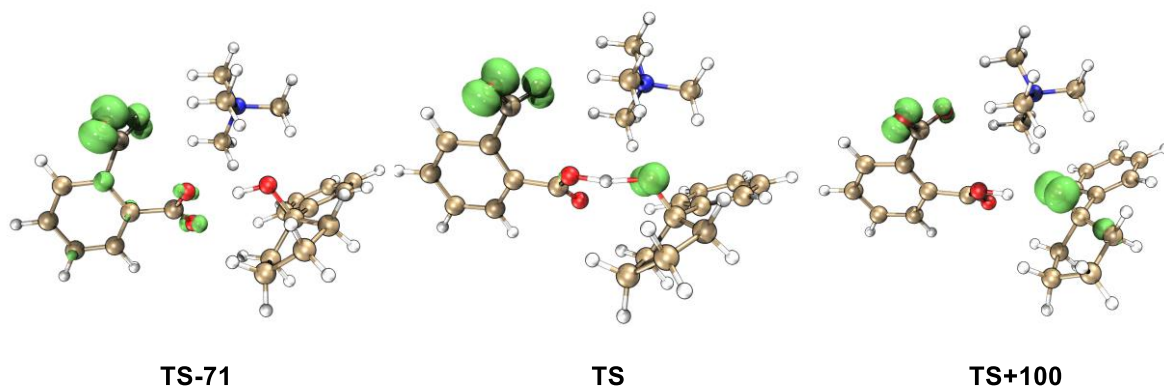
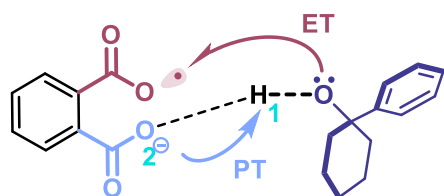
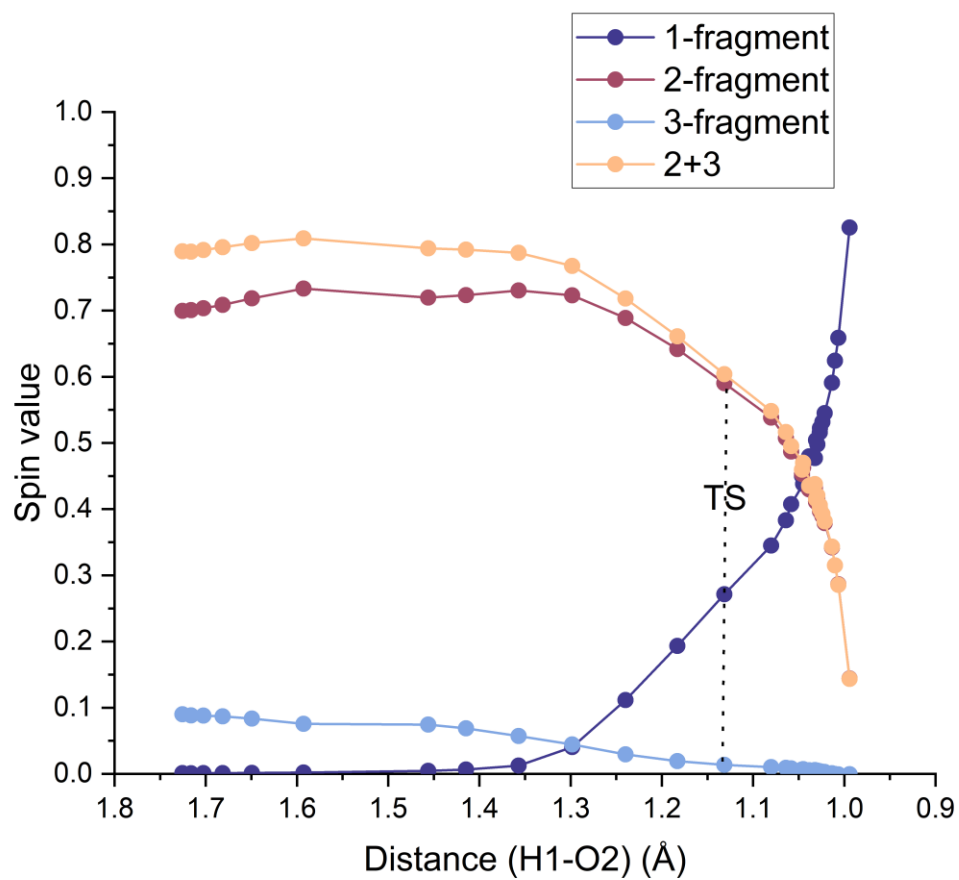


Figure S50. Spin value analysis pictures of open-shell singlet transition states TS, TS-71 and TS+100.
(green, single electron distribution)

9.3.3 TDRA-1-induced ring-opening bromination of six-membered cycloalkanol.



■ 1-fragment ■ 2-fragment ■ 3-fragment



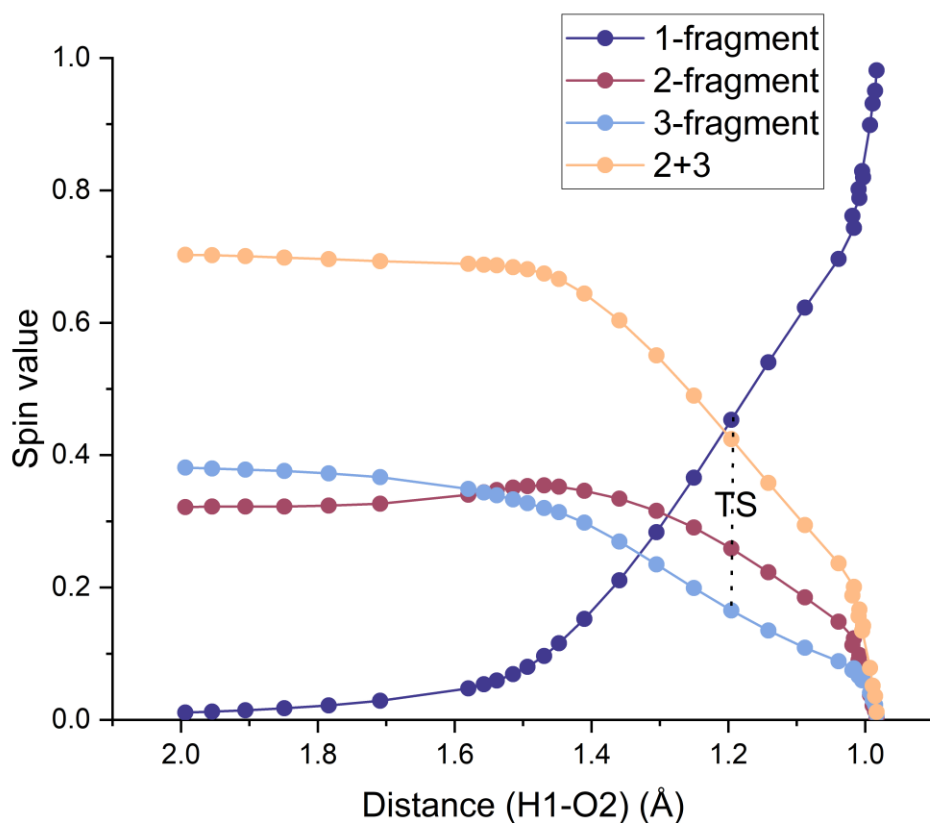


Figure S53. Selected IRC coordinates structure of the open-shell singlet transition state TS to show the change in the spin value of the 1, 2 and 3 fragments

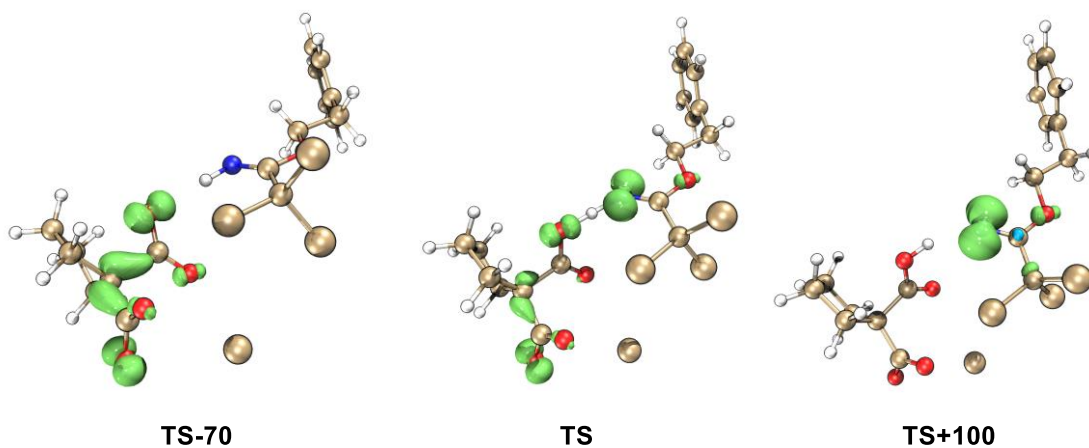


Figure S54. Spin value analysis pictures of open-shell singlet transition states TS, TS-70 and TS+100. (green, single electron distribution)

9.3.5. TDRA-3-induced C(sp³)-H amination reaction.

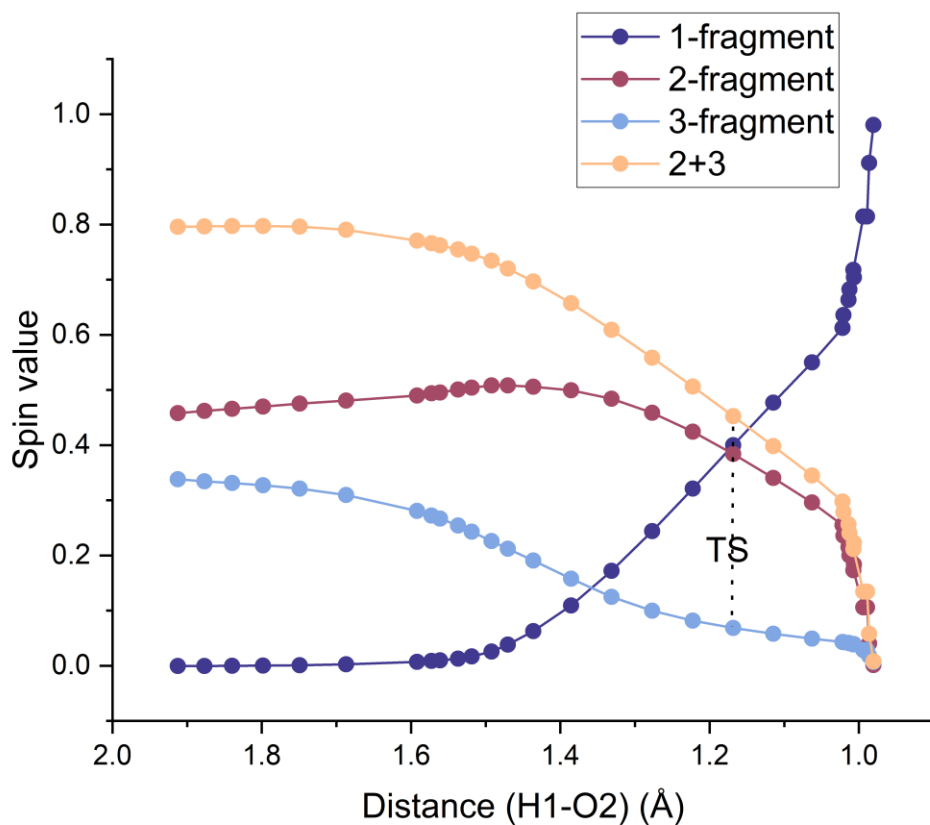
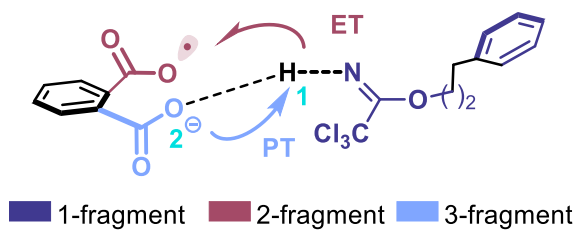


Figure S55. Selected IRC coordinates structure of the open-shell singlet transition state TS to show the change in the spin value of the 1, 2 and 3 fragments

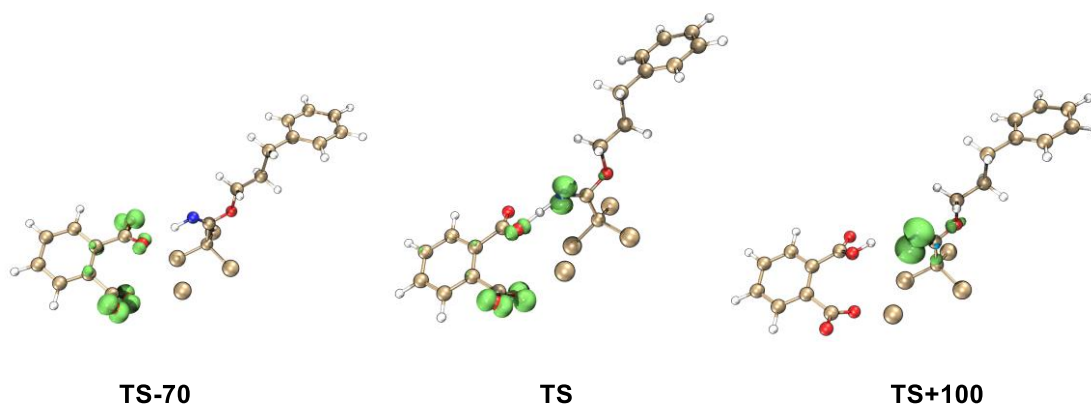
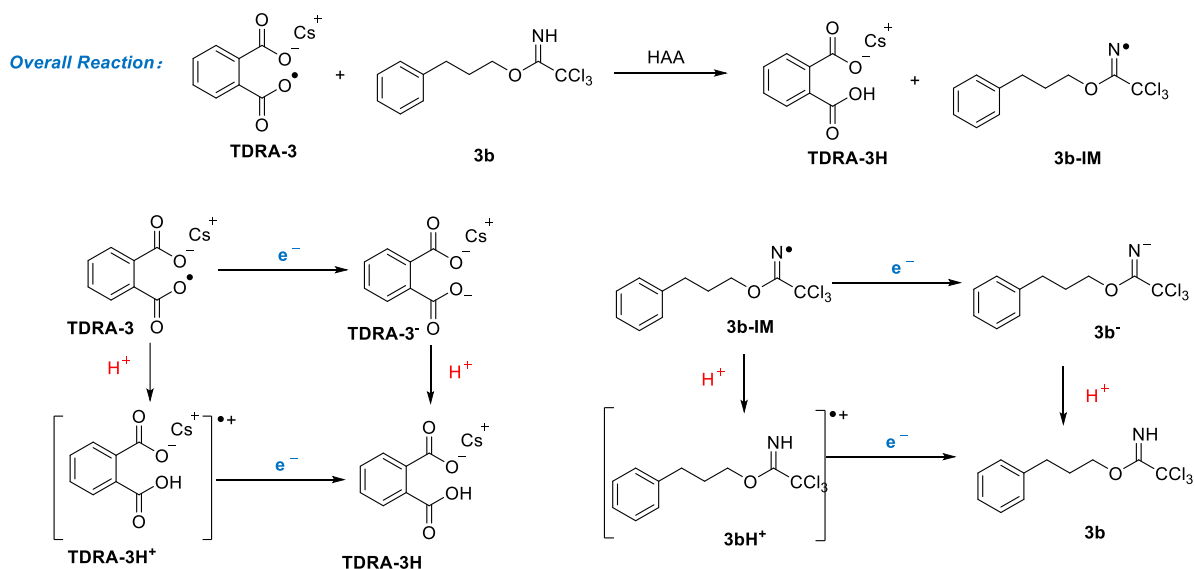


Figure S56. Spin value analysis pictures of open-shell singlet transition states TS, TS-70 and TS+100. (green, single electron distribution)

9.4 Asynchronicity Factor

In order to quantify the asynchronicity in the electron and proton transfer in the concerted HAA process, we have computed the asynchronicity factor (η) proposed by Srnec and coworkers⁸¹. η has been computed for HAA from substrates (**3a-b** and **1a, 1e, 1b**) by all TDRAs, according to **Scheme S5-S7**, which are based on the original work reported in ref. 81. In all cases, we calculate a positive value for η , which indicates asynchronicity in favor of electron-transfer.



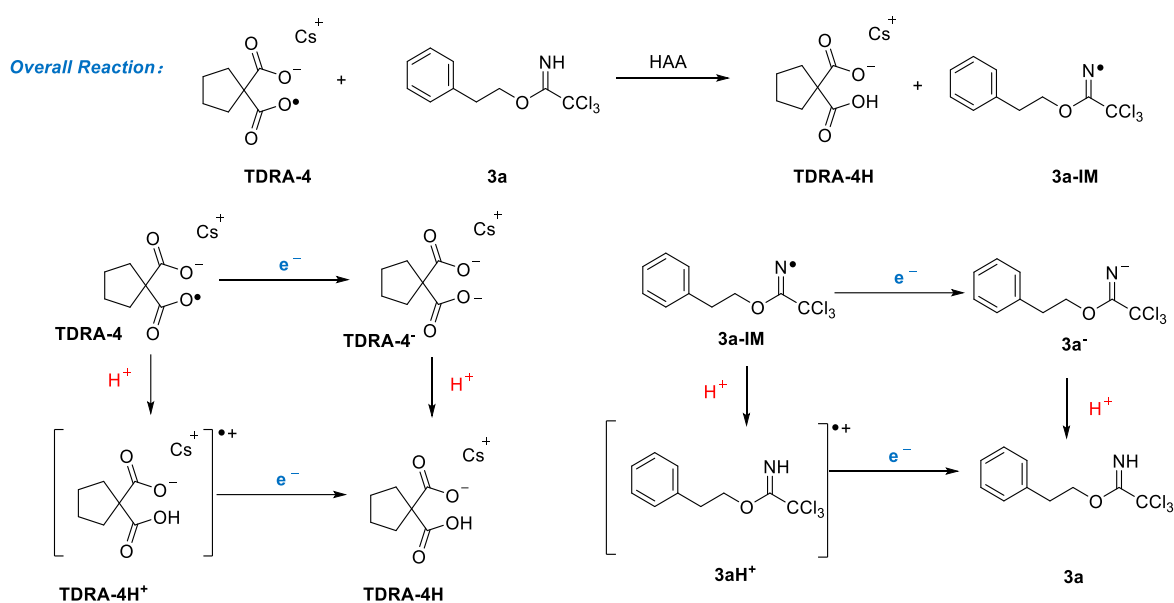
$$\text{Asynchronicity Factor } (\eta) = \frac{1}{\sqrt{2}} [-G(\text{TDRA-3}^-) + G(3b^-) + G(\text{TDRA-3H}^+) - G(3bH^+)]$$

Scheme S5. Species relevant for computing asynchronicity factor. $G(\text{species})$ refers to the Gibbs free energy of the relevant species. **[3b-r]** refers to the usual radical product after HAA, **[3bH $^+$]** is the substrate structure, **3b** oxidized by 1-electron, and **[3b $^-$]** is the substrate structure after deprotonating the acidic proton from the X-H bond.

$\eta = 64$ mV (Calculated asynchronicity factors (η) in mV, computed using Gibbs free energies of species shown in **Table S18**).

Table S18. Solution phase Gibbs free energies, $G(\text{sol})/\text{Hartree}$ for stationary points involved in **Scheme S5** for the reaction of **TDRA-3** and **3b** computed at B3LYP/6-311++G(d,p)/SMD(solvent)//B3LYP/6-31+G(d) of theory (T=298K).

File Description	$G(\text{DCE})/\text{a.u.}$
TDRA-3 $^-$	-628.716349
TDRA-3H $^+$	-628.967333
3b $^-$	-1936.557348
3bH $^+$	-1936.811653



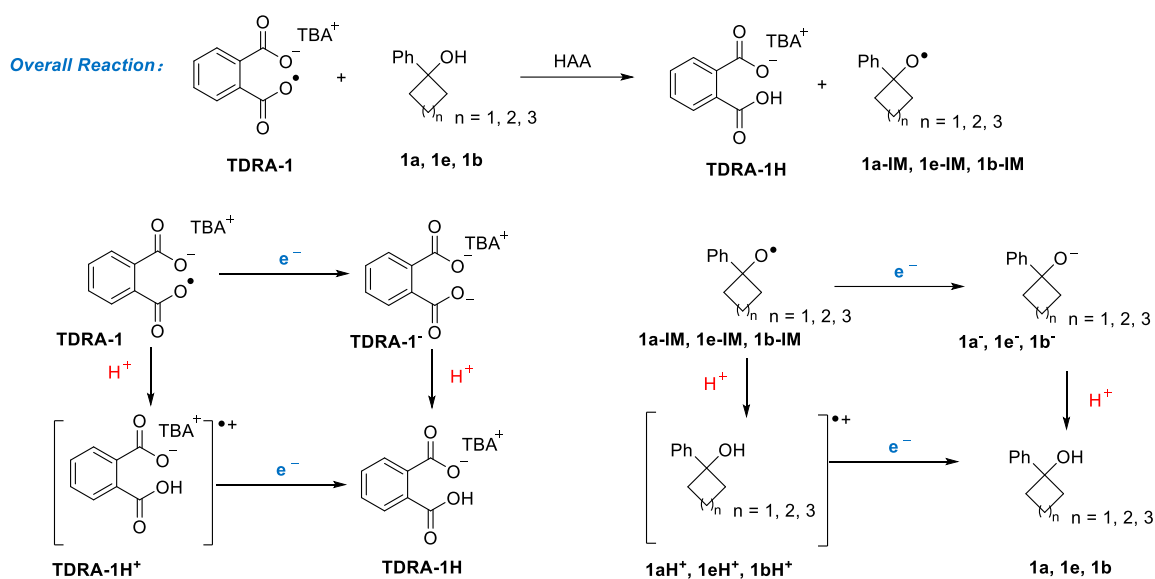
$$\text{Asynchronicity Factor } (\eta) = \frac{1}{\sqrt{2}} [-G(\text{TDRA-4}^{\bullet-}) + G(\text{3a}^{\bullet+}) + G(\text{TDRA-4H}^{\bullet+}) - G(\text{3aH}^{\bullet+})]$$

Scheme S6. Species relevant for computing asynchronicity factor. $G(\text{species})$ refers to the Gibbs free energy of the relevant species. $[\mathbf{3a-r}]$ refers to the usual radical product after HAA, $[\mathbf{3aH}^{\bullet+}]$ is the substrate structure, $\mathbf{3a}$ oxidized by 1-electron, and $[\mathbf{3a}^{\bullet-}]$ is the substrate structure after deprotonating the acidic proton from the X–H bond.

$\eta = 381$ mV (Calculated asynchronicity factors (η) in mV, computed using Gibbs free energies of species shown in **Table S19**).

Table S19. Solution phase Gibbs free energies, $G(\text{sol})/\text{Hartree}$ for stationary points involved in **Scheme S6** for the reaction of **TDRA-2** and **3a** computed at B3LYP/6-311++G(d,p)/SMD(solvent)//B3LYP/6-31+G(d) of theory (T=298K).

File Description	$G(\text{DCE})/\text{a.u.}$
TDRA-4 ^{•-}	-592.968588
TDRA-4H ^{•+}	-593.199316
3a ^{•+}	-1897.25516
3aH ^{•+}	-1897.50571



Scheme S7. Species relevant for computing asynchronicity factor. $G(\text{species})$ refers to the Gibbs free energy of the relevant species. For example, $[\mathbf{1a-r}]$ refers to the usual radical product after HAA, $[\mathbf{1aH}^+]$ is the substrate structure, $\mathbf{1a}$ oxidized by 1-electron, and $[\mathbf{1a}^-]$ is the substrate structure after deprotonating the acidic proton from the X–H bond.

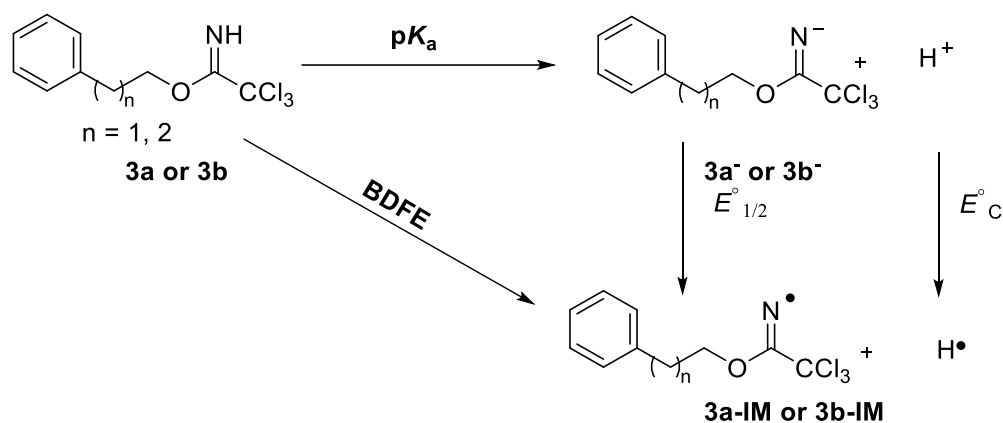
Table S20. Calculated asynchronicity factors (η) in mV, computed using Gibbs free energies of species shown in **Table S21**.

Reaction	η (mV)
TDRA-1+1a	123
TDRA-1+1e	180
TDRA-1+1b	229

Table S21. Solution phase Gibbs free energies, $G(\text{sol})/\text{Hartree}$ for stationary points involved in **Scheme S7** for the reaction of **TDRA-1** and **substrates (1a, 1e or 1b)** computed at B3LYP/6-311++G(d,p)/SMD(solvent)//B3LYP/6-31+G(d) of theory (T=298K).

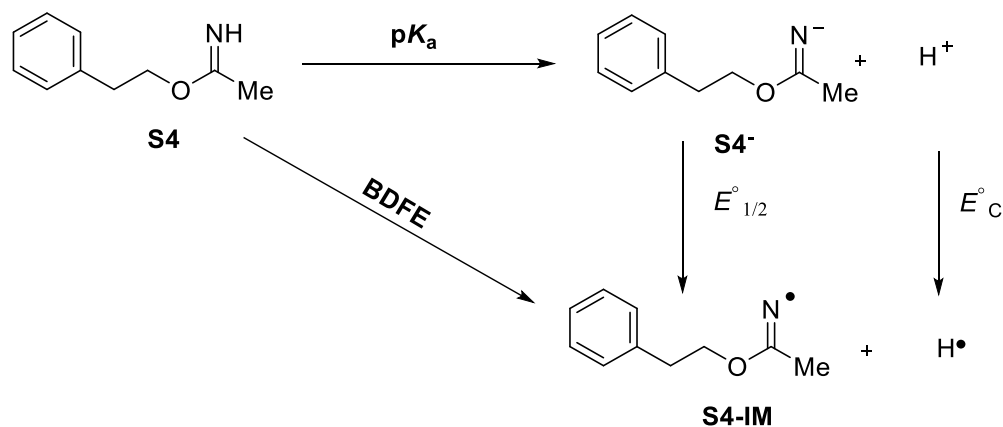
File Description	$G(\text{DCE})/\text{a.u.}$
TDRA-1 ⁻	-1294.378185
TDRA-1H ⁺	-1294.644208
1a ⁻	-462.976262
1aH ⁺	-463.248667
1e ⁻	-502.299901
1eH ⁺	-502.575287
1b ⁻	-541.606444
1bH ⁺	-541.884382

9.5 BDFE



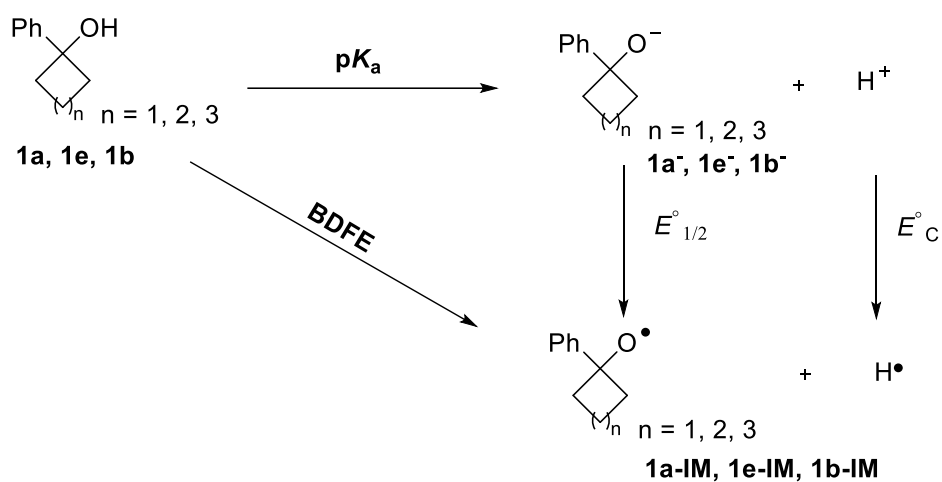
$$\text{BDFE (kcal/mol)} = 23.06 E^{\circ} (\text{R}^{\bullet}/\text{R}^-) + 1.37 \text{p}K_a (\text{RH}/\text{R}^-) + 23.06 E^{\circ} (\text{H}^+/\text{H}^{\bullet})$$

Scheme S8. The thermodynamic cycle separates the BDFE of an R–H bond into two measurable values.⁸²



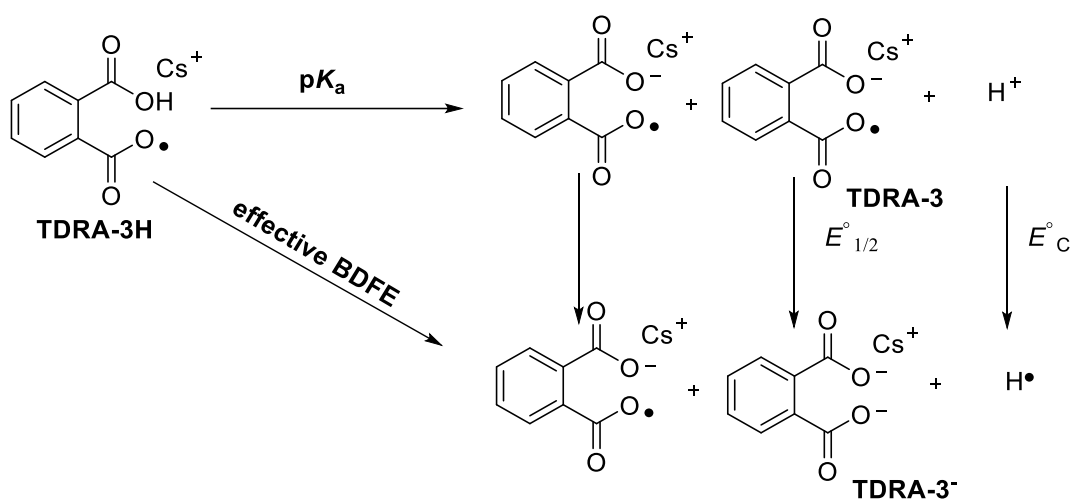
$$\text{BDFE (kcal/mol)} = 23.06 E^{\circ} (\text{R}^{\bullet}/\text{R}^-) + 1.37 \text{p}K_a (\text{RH}/\text{R}^-) + 23.06 E^{\circ} (\text{H}^+/\text{H}^{\bullet})$$

Scheme S9. The thermodynamic cycle separates the BDFE of an R–H bond into two measurable values.



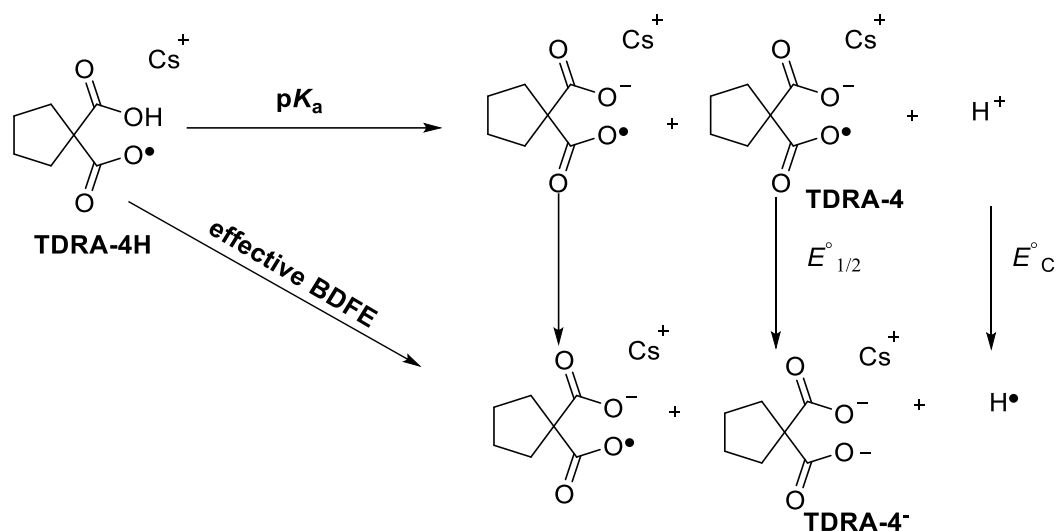
$$\text{BDFE (kcal/mol)} = 23.06 E^\circ (\text{R}^\bullet/\text{R}^-) + 1.37 \text{p}K_a (\text{RH}/\text{R}^-) + 23.06 E^\circ (\text{H}^+/\text{H}^\bullet)$$

Scheme S10. The thermodynamic cycle separates the BDFE of an R–H bond into two measurable values.



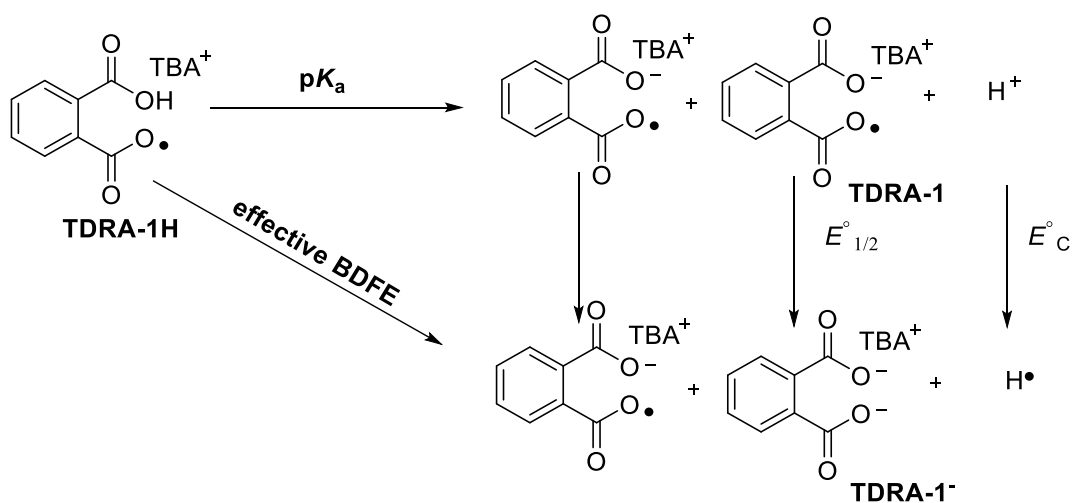
$$\text{BDFE (kcal/mol)} = 23.06 E^\circ (\text{Ox}^\bullet/\text{Ox}) + 1.37 \text{p}K_a (\text{BH}/\text{B}^-) + 23.06 E^\circ (\text{H}^+/\text{H}^\bullet)$$

Scheme S11. The thermodynamic cycle separates the BDFE of an R–H bond into two measurable values. Reagent pair and its effective BDFE.



$$\text{BDFE (kcal/mol)} = 23.06 E^\circ (\text{Ox}^{\bullet+}/\text{Ox}) + 1.37 \text{ pKa} (\text{BH}/\text{B}^-) + 23.06 E^\circ (\text{H}^+/\text{H}^\bullet)$$

Scheme S12. The thermodynamic cycle separates the BDFE of an R–H bond into two measurable values. Reagent pair and its effective BDFE.



$$\text{BDFE (kcal/mol)} = 23.06 E^\circ (\text{Ox}^{\bullet+}/\text{Ox}) + 1.37 \text{ pKa} (\text{BH}/\text{B}^-) + 23.06 E^\circ (\text{H}^+/\text{H}^\bullet)$$

Scheme S13. The thermodynamic cycle separates the BDFE of an R–H bond into two measurable values. Reagent pair and its effective BDFE.

Table S22. A series of O/N–H BDFEs and effective BDFEs are tabulated to show the balancing effect between pKa and E° . E° is computed using Gibbs free energies of species shown in **Table S23** The free energy change for the reference reaction in the standard hydrogen electrode (SHE). In this study, the value -4.44 V is consistently used in all calculations. The pKa datas are based on <http://pka.luozsgroup.com/>.⁸³

File Description	E° (eV)	pKa	BDFE
TDRA-1 ⁻	0.32	22.73	93

TDRA-2	0.42	13.80	84
TDRA-3	0.73	14.65	92
1a	-0.24	22.89	81
1e	-0.26	23.57	81
1b	-0.28	24.11	81
3a	0.07	19.70	83
3b	0.04	20.49	84
S4	-0.90	23.52	66

Table S23. The Gibbs free energy potential surface for the oxidants and substrates computed at M052X/6-31G(d)/SMD(Acetonitrile)//B3LYP/6-31+G(d) level of theory.

File Description	$\Delta G(\text{MeCN})$
TDRA-1⁻	0.17484999999878
TDRA-2	0.178741999999829
TDRA-3	0.189995999999951
1a	0.154302999999970
1e	0.153442999999925
1b	0.152872000000002
3a	0.165703999999778
3b	0.164452999999867
S4	0.130210999999917

Based on the above observations, we performed an additional assessment of the thermodynamic driving force for the PCET process. Mayer emphasized that the capability of a specific oxidant/base pair to serve as a formal hydrogen radical (H•) acceptor could be quantified through an effective bond strength, denoted as the BDFE, which can be derived from the pK_a and reduction potential. In our proposed mechanism, the relevant oxidant is the carboxylic radical subunit in the TDRA while the Brønsted base is the carboxylate anion subunit. Therefore, we calculated the effective bond strengths of TDRA (ranging from 84 to 93 kcal/mol) and O/N–H BDFEs in cycloalkanols and imidates (81 kcal/mol and 83–84 kcal/mol). Remarkably, in all cases wherein the effective BDFEs of the TDRA approach or exceed that of the substrates, the reactions are successful and afford the expected products. The reaction of the imidate bearing a methyl group **S5** furnish no product, because effective BDFEs of the TDRA are much greater than 66 kcal/mol (N–H BDFE = 66 kcal/mol in the **S5**). These energetic correlations offer further proofs that the PCET processes are actually involved in the two TDRA-mediated transformations.

10. References

- (1) Griffith, J. C.; Jones, K. M.; Picon, S.; Rawling, M. J.; Kariuki, B. M.; Campbell, M.; Tomkinson, N. C. O. Alkene Syn Dihydroxylation with Malonoyl Peroxides. *J. Am. Chem. Soc.* **2010**, *132*, 14409–14411.
- (2) Gan, S.; Yin, J.; Yao, Y.; Liu, Y.; Chang, D.; Zhu, D.; Shi, L. Metal- and Additive-Free Oxygen-Atom Transfer Reaction: An Efficient and Chemoselective Oxidation of Sulfides to Sulfoxides with Cyclic Diacyl Peroxides. *Org. Biomol. Chem.* **2017**, *15*, 2647–2654.
- (3) Concepcion, J. J.; Brennaman, M. K.; Deyton, J. R.; Lebedeva, N. V.; Forbes, M. D. E.; Papanikolas, J. M.; Meyer, T. J. Excited-State Quenching by Proton-Coupled Electron Transfer. *J. Am. Chem. Soc.* **2007**, *129*, 6968–6969.
- (4) Irebo, T.; Reece, S. Y.; Sjödin, M.; Nocera, D. G.; Hammarström, L. Proton-Coupled Electron Transfer of Tyrosine Oxidation: Buffer Dependence and Parallel Mechanisms. *J. Am. Chem. Soc.* **2007**, *129*, 15462–15464.
- (5) Morris, W. D.; Mayer, J. M. Separating Proton and Electron Transfer Effects in Three-Component Concerted Proton-Coupled Electron Transfer Reactions. *J. Am. Chem. Soc.* **2017**, *139*, 10312–10319.
- (6) Markle, T. F.; Mayer, J. M. Concerted Proton–Electron Transfer in Pyridylphenols: The Importance of the Hydrogen Bond. *Angew Chem Int Ed* **2008**, *47*, 738–740.
- (7) Chalkley, M. J.; Garrido-Barros, P.; Peters, J. C. A Molecular Mediator for Reductive Concerted Proton-Electron Transfers via Electrocatalysis. *Science* **2020**, *369*, 850–854.
- (8) Hankache, J.; Hanss, D.; Wenger, O. S. Hydrogen-Bond Strengthening upon Photoinduced Electron Transfer in Ruthenium–Anthraquinone Dyads Interacting with Hexafluoroisopropanol or Water. *J. Phys. Chem. A* **2012**, *116*, 3347–3358.
- (9) Darcy, J. W.; Kolmar, S. S.; Mayer, J. M. Transition State Asymmetry in C–H Bond Cleavage by Proton-Coupled Electron Transfer. *J. Am. Chem. Soc.* **2019**, *141*, 10777–10787.
- (10) Tarantino, K. T.; Liu, P.; Knowles, R. R. Catalytic Ketyl-Olefin Cyclizations Enabled by Proton-Coupled Electron Transfer. *J. Am. Chem. Soc.* **2013**, *135*, 10022–10025.
- (11) Warren, J. J.; Mayer, J. M. Proton-Coupled Electron Transfer Reactions at a Heme-Propionate in an Iron-Protoporphyrin-IX Model Compound. *J. Am. Chem. Soc.* **2011**, *133*, 8544–8551.
- (12) Walling, C.; Bristol, D. ..Delta.-Chloro Alcohols and Tetrahydrofurans from Primary and Secondary Alkyl Hypochlorites. *J. Org. Chem.* **1972**, *37*, 3514–3516.
- (13) Zlotorzynska, M.; Zhai, H.; Sammis, G. M. Chemoselective Oxygen-Centered Radical Cyclizations onto Silyl Enol Ethers. *Org. Lett.* **2008**, *10*, 5083–5086.
- (14) Pasto, D. J.; Cottard, F. Demonstration of the Synthetic Utility of the Generation of Alkoxy Radicals by the Photo-Induced Homolytic Dissociation of Alkyl 4-Nitrobenzenesulfenates. *Tetrahedron Letters* **1994**, *35*, 4303–4306.
- (15) De Armas, P.; Francisco, C. G.; Suárez, E. Reagents with Hypervalent Iodine: Formation of Convenient Chiral Synthetic Intermediates by Fragmentation of Carbohydrate Anomeric Alkoxy Radicals. *Angew. Chem. Int. Ed. Engl.* **1992**, *31*, 772–774.
- (16) Barton D. H. R.; Beaton J. M.; Geller L. E.; et al. A New Photochemical Reaction. *J. Am. Chem. Soc.* **1960**, *82*: 2640–2641.
- (17) Kochi J. K. Chemistry of Alkoxy Radicals: Cleavage Reactions. *J. Am. Chem. Soc.* **1962**, *84*: 1193–1197.
- (18) Bao, X.; Wang, Q.; Zhu, J. Dual Photoredox/Copper Catalysis for the Remote C(Sp³)–H Functionalization of Alcohols and Alkyl Halides by *N*-Alkoxyppyridinium Salts. *Angew Chem Int Ed* **2019**, *58*, 2139–2143.
- (19) Guo, J.; Hu, A.; Chen, Y.; Sun, J.; Tang, H.; Zuo, Z. Photocatalytic C–C Bond Cleavage and

- Amination of Cycloalkanols by Cerium(III) Chloride Complex. *Angew Chem Int Ed* **2016**, *55*, 15319–15322.
- (20) Kananovich, D. G.; Konik, Y. A.; Zubrytski, D. M.; Järving, I.; Lopp, M. Simple Access to β -Trifluoromethyl-Substituted Ketones via Copper-Catalyzed Ring-Opening Trifluoromethylation of Substituted Cyclopropanols. *Chem. Commun.* **2015**, *51*, 8349–8352.
- (21) Yayla, H. G.; Wang, H.; Tarantino, K. T.; Orbe, H. S.; Knowles, R. R. Catalytic Ring-Opening of Cyclic Alcohols Enabled by PCET Activation of Strong O–H Bonds. *J. Am. Chem. Soc.* **2016**, *138*, 10794–10797.
- (22) Huang, F.-Q.; Xie, J.; Sun, J.-G.; Wang, Y.-W.; Dong, X.; Qi, L.-W.; Zhang, B. Regioselective Synthesis of Carbonyl-Containing Alkyl Chlorides via Silver-Catalyzed Ring-Opening Chlorination of Cycloalkanols. *Org. Lett.* **2016**, *18*, 684–687.
- (23) Herron, A. N.; Liu, D.; Xia, G.; Yu, J.-Q. δ -C–H Mono- and Dihalogenation of Alcohols. *J. Am. Chem. Soc.* **2020**, *142*, 2766–2770.
- (24) Barthelemy, A.; Tuccio, B.; Magnier, E.; Dagousset, G. Alkoxy Radicals Generated under Photoredox Catalysis: A Strategy for anti-Markovnikov Alkoxylation Reactions. *Angew Chem Int Ed* **2018**, *57*, 13790–13794.
- (25) Hofmann A. W. Ueber die Einwirkung des Broms in alkalischer Lösung auf die Amine. *Berichte der deutschen chemischen Gesellschaft*, **1883**, *16*, 558-560.
- (26) Löffler K.; Freytag C. Über eine neue Bildungsweise von *N*-alkylierten Pyrrolidinen. *Berichte der deutschen chemischen Gesellschaft*, **1909**, *42*, 3427-3431.
- (27) Hernández R.; Rivera A.; Salazar J A.; et al. Nitroamine Radicals as Intermediates in the Functionalization of Non-Activated Carbon Atoms. *Journal of the Chemical Society, Chemical Communications*, **1980**, *20*, 958-959.
- (28) Martínez C.; Muñoz K. An Iodine-Catalyzed Hofmann–Löffler Reaction[J]. *Angew Chem Int Ed.* **2015**, *54*, 8287-8291.
- (29) Wappes E. A.; Fosu S. C.; Chopko T. C.; et al. Triiodide-Mediated δ -Amination of Secondary C–H Bonds. *Angew Chem Int Ed.* **2016**, *55*, 9974-9978.
- (30) Edwards O. E.; Rosich R. S. Photolysis of a Medium-Ring Nitrosamide. *Canadian Journal of Chemistry*, **1967**, *45*, 1287-1290.
- (31) Newcomb M.; Marquardt D. J.; Deeb T. M. *N*-Hydroxypyridine-2-thione Carbamates. v. Syntheses of Alkaloid Skeletons by Aminium Cation Radical Cyclizations. *Tetrahedron*, **1990**, *46*, 2329-2344.
- (32) Boivin J.; Fouquet E.; Schiano A-M.; et al. Iminyl Radicals: Part III. Further Synthetically Useful Sources of Iminyl Radicals. *Tetrahedron*, **1994**, *50*, 1769-1776.
- (33) Davies J.; Sheikh N. S.; Leonori D. Photoredox Imino Functionalizations of Olefins[J]. *Angew Chem Int Ed.* **2017**, *56*, 13361-13365.
- (34) Guin J.; Mück-Lichtenfeld C.; Grimme S.; et al. Radical Transfer Hydroamination with Aminated Cyclohexadienes Using Polarity Reversal Catalysis: Scope and Limitation. *J. Am. Chem. Soc.* **2007**, *129*, 4498-4503.
- (35) Kitagawa O.; Miyaji S.; Yamada Y.; et al. Iodine Atom Transfer [3+2] Cycloaddition Reaction with Electron-Rich Alkenes Using *N*-Tosyliodoaziridine Derivatives as Novel Azahomoallyl Radical Precursors. *The Journal of Organic Chemistry*, **2003**, *68*, 3184-3189.
- (36) Groendyke B. J.; AbuSalim D. I.; Cook S. P. Iron-Catalyzed, Fluoroamide-Directed C–H Fluorination. *J. Am. Chem. Soc.* **2016**, *138*, 12771-12774.
- (37) Li Z.; Wang Q.; Zhu J. Copper-Catalyzed Arylation of Remote C(sp³)–H Bonds in Carboxamides and Sulfonamides. *Angew Chem Int Ed.* **2018**, *57*, 13288-13292.
- (38) Zhang Z.; Stateman L. M.; Nagib D. A. δ C–H (Hetero)arylation via Cu-Catalyzed Radical Relay.

Chemical Science, **2019**, *10*, 1207-1211.

(39) Liu Z.; Xiao H.; Zhang B.; et al. Copper-Catalyzed Remote C(sp³)-H Trifluoromethylation of Carboxamides and Sulfonamides. *Angew Chem Int Ed.* **2019**, *58*, 2510-2513.

(40) Snee, R. A.; Matheny, N. P. Mechanisms of Substitution at Unactivated Carbon Atoms. *J. Am. Chem. Soc.* **1964**, *86*, 5503-5511.

(41) Alvi, S.; Singleton, D. A. Energy Read-out as a Probe of Kinetically Hidden Transition States. *Org. Lett.* **2021**, *23*, 2174-2177.

(42) Zhao, R.; Yao, Y.; Zhu, D.; Chang, D.; Liu, Y.; Shi, L. Visible-Light-Enhanced Ring Opening of Cycloalkanols Enabled by Brønsted Base-Tethered Acyloxy Radical Induced Hydrogen Atom Transfer-Electron Transfer. *Org. Lett.* **2018**, *20*, 1228-1231.

(43) Bosnidou, A. E.; Duhamel, T.; Muñoz, K. Detection of the Elusive Nitrogen-Centered Radicals from Catalytic Hofmann-Löffler Reactions. *Eur. J. Org. Chem.* **2020**, *2020*, 6361-6365.

(44) Ingold, K. U.; Pratt, D. A. Advances in Radical-Trapping Antioxidant Chemistry in the 21st Century: A Kinetics and Mechanisms Perspective. *Chem. Rev.* **2014**, *114*, 9022-9046

(45) Uyanik, M.; Hayashi, H.; Ishihara, K. High-Turnover Hypoiodite Catalysis for Asymmetric Synthesis of Tocopherols. *Science* **2014**, *345*, 291-294.

(46) Wang, J.; Liu, X.; Wu, Z.; Li, F.; Zhang, M.-L.; Mi, Y.; Wei, J.; Zhou, Y.; Liu, L. Ag-Catalyzed Ring-Opening of Tertiary Cycloalkanols for C-H Functionalization of Cyclic Aldimines. *Chem. Commun.* **2021**, *57*, 1506-1509.

(47) Xu, Z.-M.; Li, H.-X.; Young, D. J.; Zhu, D.-L.; Li, H.-Y.; Lang, J.-P. Exogenous Photosensitizer-, Metal-, and Base-Free Visible-Light-Promoted C-H Thiolation via Reverse Hydrogen Atom Transfer. *Org. Lett.* **2019**, *21*, 237-241.

(48) Gaussian 09, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2010.

(49) Vosko, S. H.; Wilk, L.; Nusair, M. Accurate Spin-Dependent Electron Liquid Correlation Energies for Local Spin Density Calculations: A Critical Analysis. *Can. J. Phys.* **1980**, *58*, 1200-1211.

(50) Becke, A. D. Density-Functional Thermochemistry. III. The Role of Exact Exchange. *The Journal of Chemical Physics* **1993**, *98*, 5648-5652.

(51) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. Ab Initio Calculation of Vibrational Absorption and Circular Dichroism Spectra Using Density Functional Force Fields. *J. Phys. Chem.* **1994**, *98* (45), 11623-11627. <https://doi.org/10.1021/j100096a001>.

(52) Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron Density. *Phys. Rev. B* **1988**, *37*, 785-789.

(53) Becke, A. D. Density-Functional Exchange-Energy Approximation with Correct Asymptotic Behavior. *Phys. Rev. A* **1988**, *38*, 3098-3100.

(54) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A Consistent and Accurate *Ab Initio* Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. *J. Chem. Phys.* **2010**, *132*,

154104.

(55) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **2009**, *113*, 6378–6396.

(56) Ho, J.; Klamt, A.; Coote, M. L. Comment on the Correct Use of Continuum Solvent Models. *J. Phys. Chem. A* **2010**, *114*, 13442–13444.

(57) CYLview, 1.0b; Legault, C. Y. Université de Sherbrooke, 2009 (<http://www.cylview.org>)

(58) Parr, R. G.; Szentpály, L. V.; Liu, S. Electrophilicity Index. *J. Am. Chem. Soc.* **1999**, *121*, 1922–1924.

(59) Héberger, K.; Lopata, A. Assessment of Nucleophilicity and Electrophilicity of Radicals, and of Polar and Enthalpy Effects on Radical Addition Reactions. *J. Org. Chem.* **1998**, *63*, 8646–8653.

(60) Lu, T.; Chen, Q. Realization of Conceptual Density Functional Theory and Information-Theoretic Approach in Multiwfn Program. In *Conceptual Density Functional Theory*, WILEY-VCH GmbH: Weinheim. **2022**, 631–647.

(61) Hoffmann, G.; Tognetti, V.; Joubert, L. Electrophilicity Indices and Halogen Bonds: Some New Alternatives to the Molecular Electrostatic Potential. *J. Phys. Chem. A* **2020**, *124*, 2090–2101.

(62) Murray, J. S.; Politzer, P. The Electrostatic Potential: An Overview. *WIREs Comput Mol Sci* **2011**, *1*, 153–163.

(63) Politzer, P.; Murray, J. S. Potential as a Guide to Molecular Interactive Behavior. *Chemical Reactivity Theory*.

(64) Politzer, P.; Murray, J. S. The Fundamental Nature and Role of the Electrostatic Potential in Atoms and Molecules. *Theoretical Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta)* **2002**, *108*, 134–142.

(65) Sjöberg, P.; Murray, J. S.; Brinck, T.; Politzer, P. Average Local Ionization Energies on the Molecular Surfaces of Aromatic Systems as Guides to Chemical Reactivity. *Can. J. Chem.* **1990**, *68*, 1440–1443.

(66) Politzer, P.; Murray, J. S.; Bulat, F. A. Average Local Ionization Energy: A Review. *J Mol Model* **2010**, *16*, 1731–1742.

(67) Lu, T.; Chen, F. Multiwfn: A Multifunctional Wavefunction Analyzer. *J. Comput. Chem.* **2012**, *33*, 580–592.

(68) VMD Research. <http://www.tcbg.illinois.edu/Research/vmd>

(69) Hu, A.; Guo, J.-J.; Pan, H.; Zuo, Z. Selective functionalization of methane, ethane, and higher alkanes by cerium photocatalysis. *Science* **2018**, *361*, 668–672.

(70) Xu, W.; Ma, J.; Yuan, X.; Dai, J.; Xie, J.; Zhu, C. Synergistic Catalysis for the Umpolung Trifluoromethylthiolation of Tertiary Ethers. *Angew. Chem., Int. Ed.* **2018**, *57*, 10357–10361.

(71) Jeffrey, J. L.; Terrett, J. A.; MacMillan, D. W. C. O–H Hydrogen Bonding Promotes H-Atom Transfer from α C–H Bonds for C-Alkylation of Alcohols. *Science* **2015**, *349*, 1532–1536.

(72) Le, C.; Liang, Y.; Evans, R. W.; Li, X.; MacMillan, D. W. C. Selective C(sp³)-H Alkylation via Polarity-Match-Based Cross-Coupling. *Nature* **2017**, *547*, 79–83.

(73) Twilton, J.; Christensen, M.; DiRocco, D. A.; Ruck, R. T.; Davies, I. W.; MacMillan, D. W. C. Selective Hydrogen Atom Abstraction through Induced Bond Polarization: Direct α -Arylation of Alcohols through Photoredox, HAT, and Nickel Catalysis. *Angew. Chem., Int. Ed.* **2018**, *57*, 5369–5373.

(74) Guo, X.; Wenger, O. S. Reductive Amination by Photoredox Catalysis and Polarity-Matched Hydrogen Atom Transfer. *Angew. Chem., Int. Ed.* **2018**, *57*, 2469–2473.

(75) Shaw, M. H.; Shurtleff, V. W.; Terrett, J. A.; Cuthbertson, J. D.; MacMillan, D. W. C. Native Functionality in Triple Catalytic Cross-Coupling: C(sp³)-H Bonds as Latent Nucleophiles. *Science* **2016**, *352*, 1304–1308.

(76) Mukherjee, S.; Maji, B.; Tlahuext-Aca, A.; Glorius, F. Visible-Light-Promoted Activation of

Unactivated C(sp³)-H Bonds and Their Selective Trifluoromethylthiolation. *J. Am. Chem. Soc.* **2016**, *138*, 16200–16203.

(77) Musacchio, A. J.; Lainhart, B. C.; Zhang, X.; Naguib, S. G.; Sherwood, T. C.; Knowles, R. R. Catalytic Intermolecular Hydroaminations of Unactivated Olefins with Secondary Alkyl Amines. *Science* **2017**, *355*, 727–730.

(78) Yang, H.-B.; Feceu, A.; Martin, D. B. C. Catalyst-Controlled C–H Functionalization of Adamantanes Using Selective H-Atom Transfer. *ACS Catal.* **2019**, *9*, 5708–5715.

(79) Miller, D. C.; Choi, G. J.; Orbe, H. S.; Knowles, R. R. Catalytic Olefin Hydroamidation Enabled by Proton-Coupled Electron Transfer. *J. Am. Chem. Soc.* **2015**, *137*, 13492–13495.

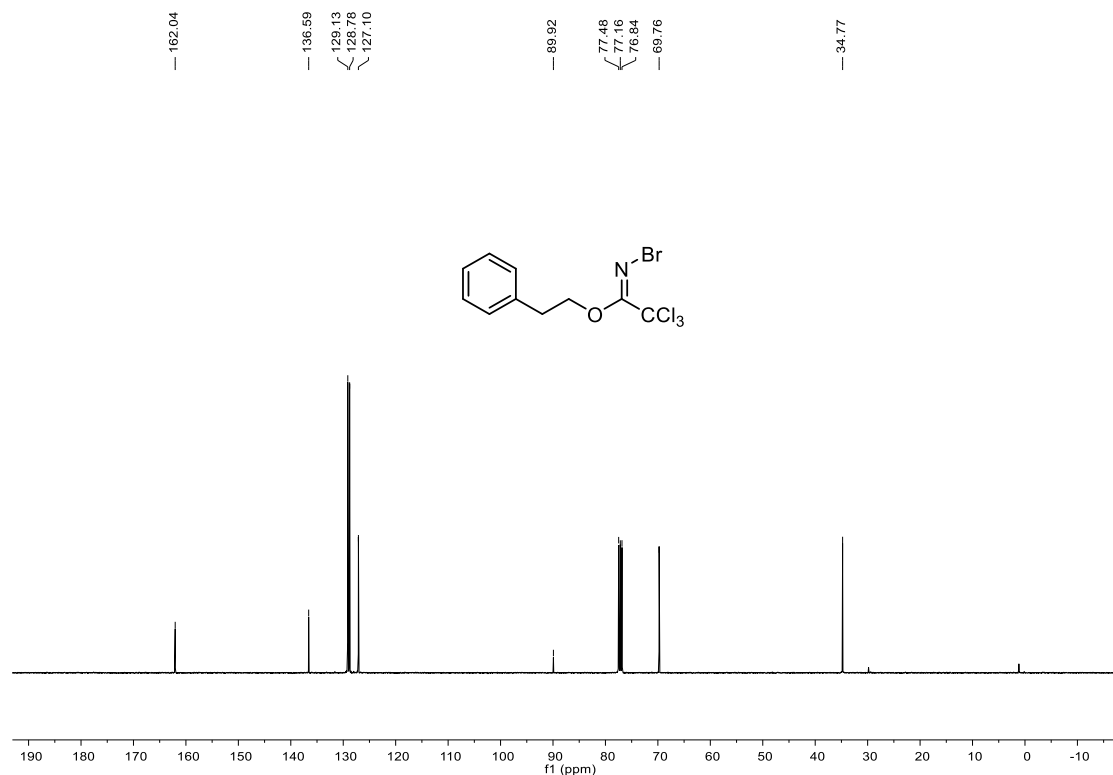
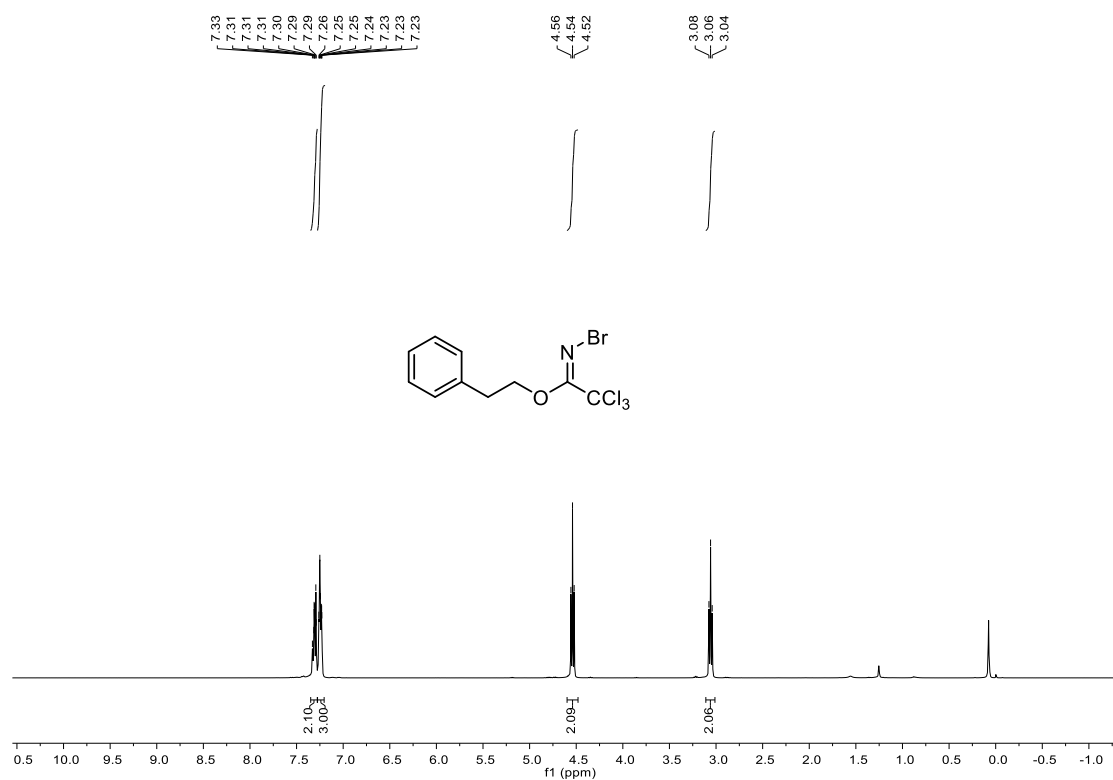
(80) Knizia, G. Intrinsic Atomic Orbitals: An Unbiased Bridge between Quantum Theory and Chemical Concepts. *J. Chem. Theory Comput.* **2013**, *9*, 4834–4843.

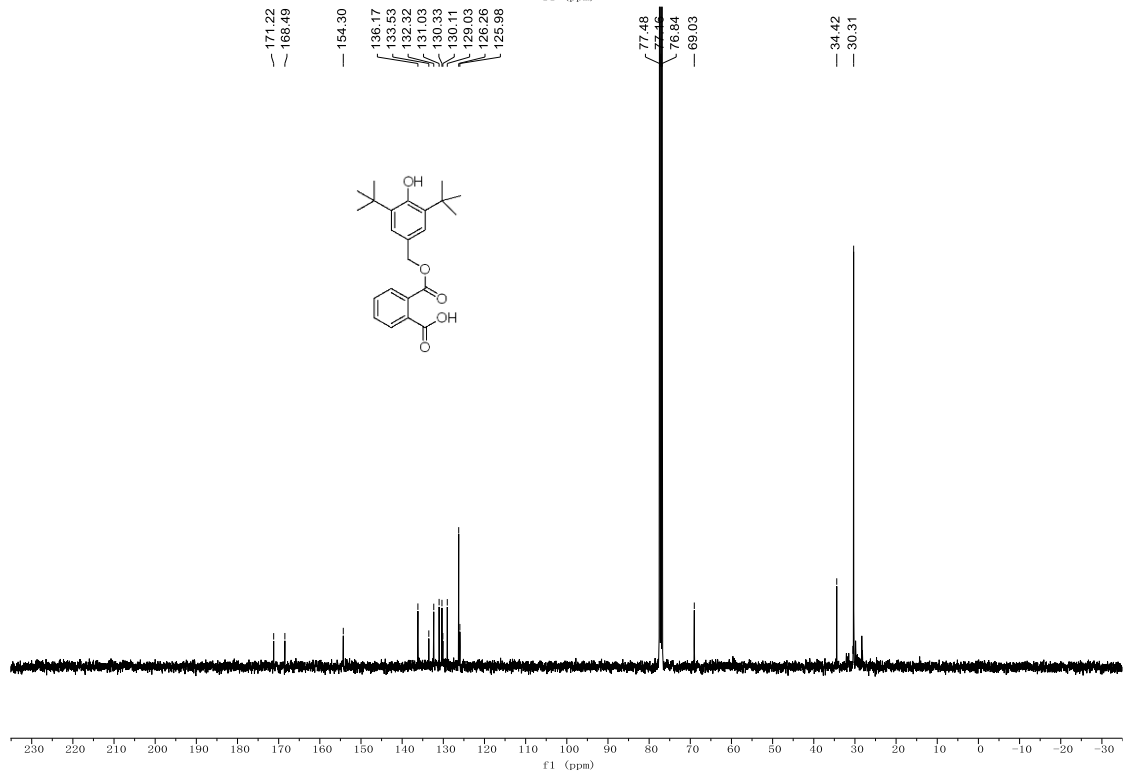
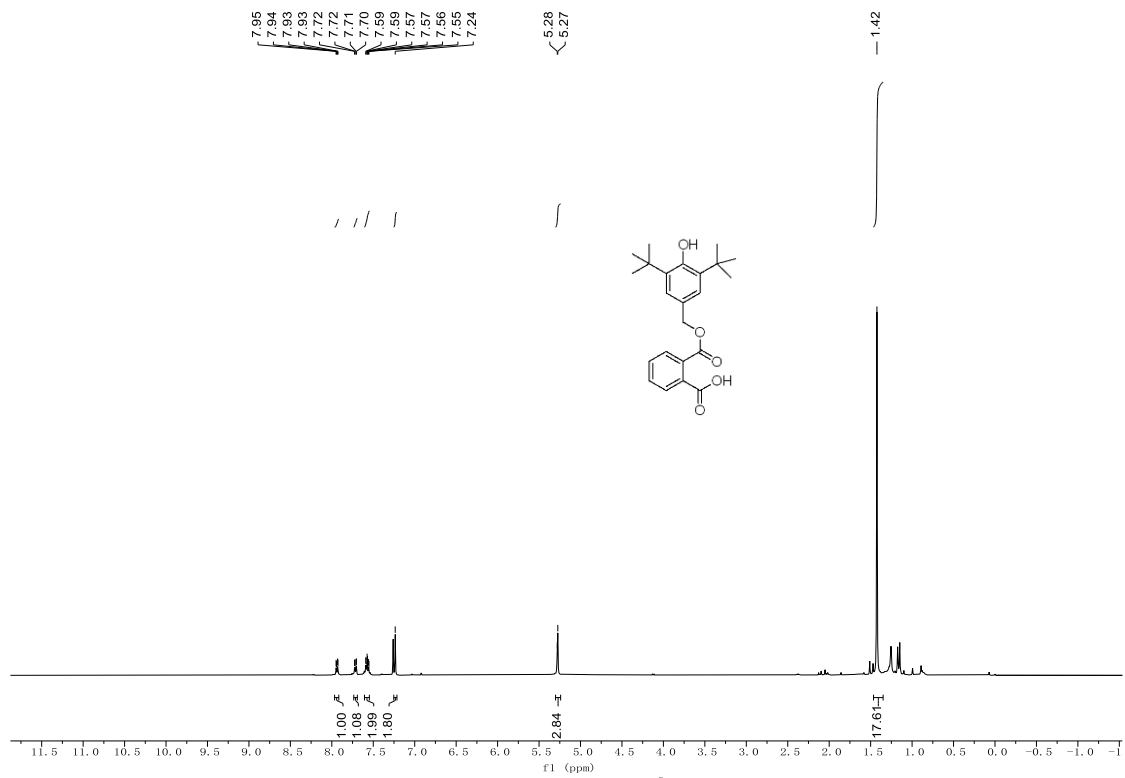
(81) Bím, D.; Maldonado-Domínguez, M.; Rulíšek, L.; Smec, M. Beyond the Classical Thermodynamic Contributions to Hydrogen Atom Abstraction Reactivity. *Proc. Natl. Acad. Sci. U.S.A.* **2018**, *115*, 10287–10294.

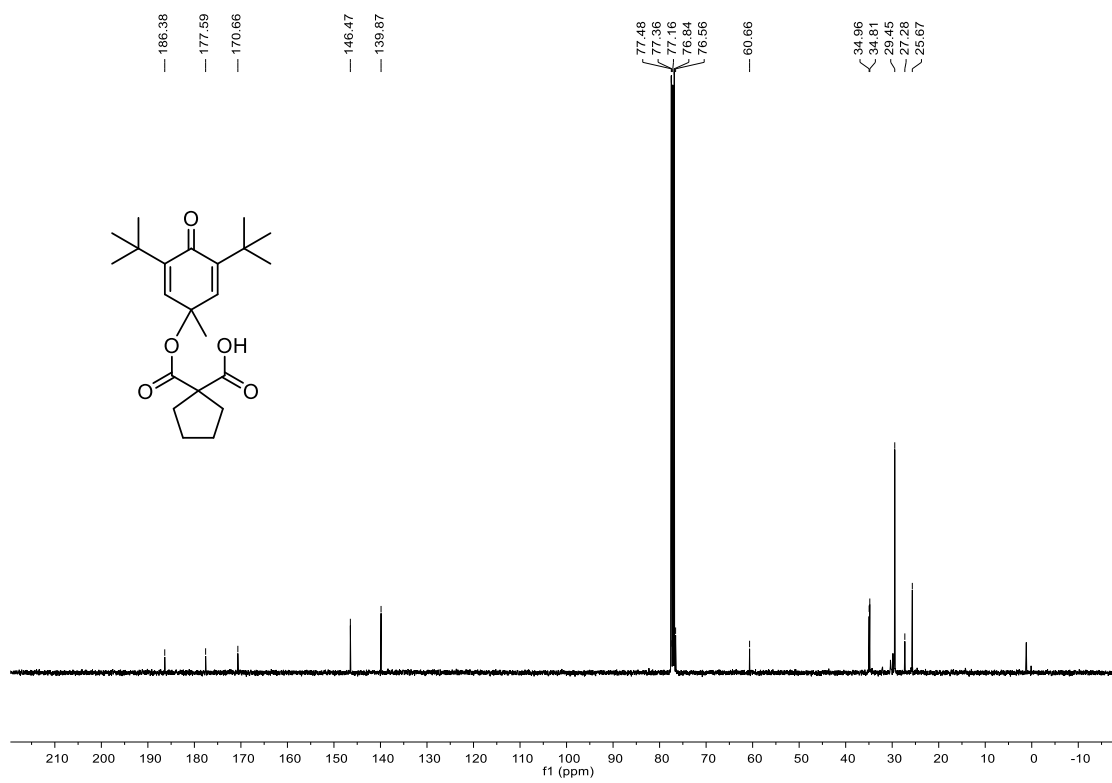
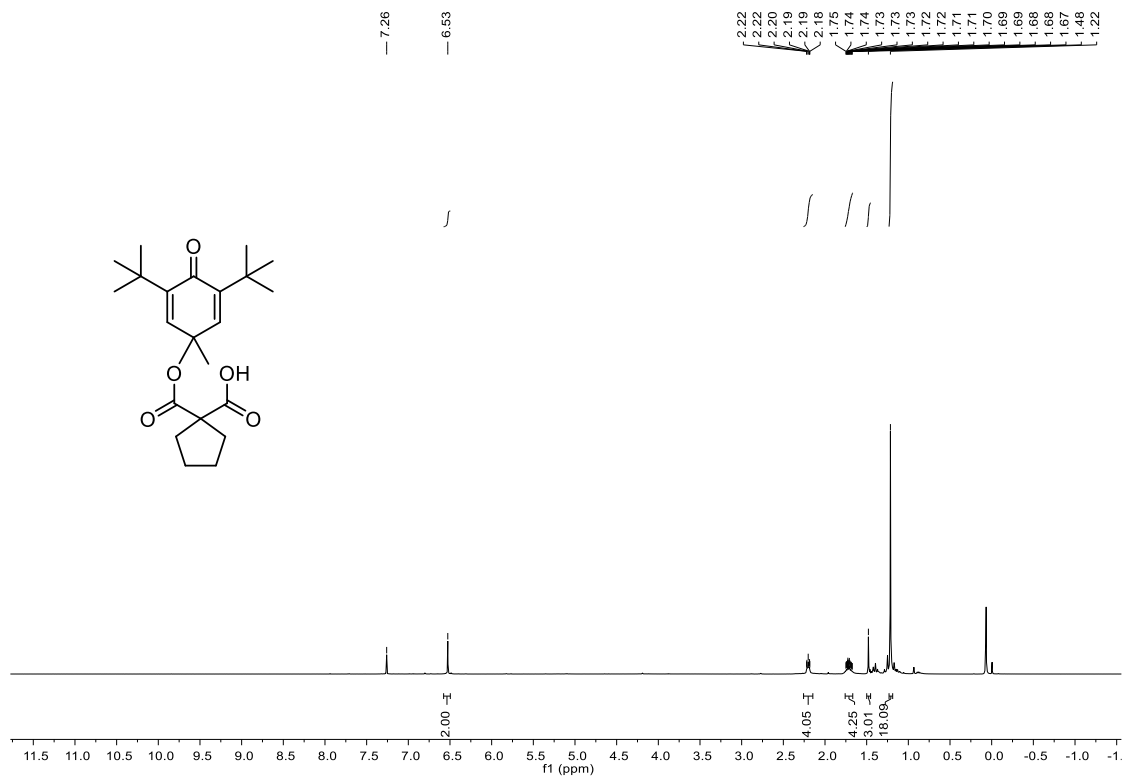
(82) Warren, J. J.; Tronic, T. A.; Mayer, J. M. Thermochemistry of Proton-Coupled Electron Transfer Reagents and Its Implications. *Chem. Rev.* **2010**, *110*, 6961–7001.

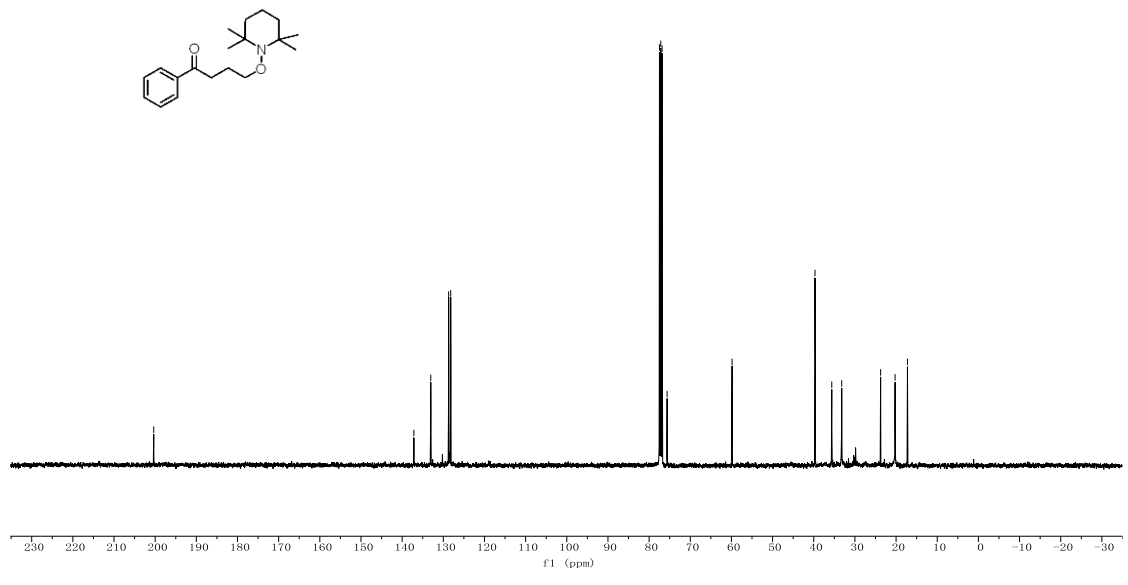
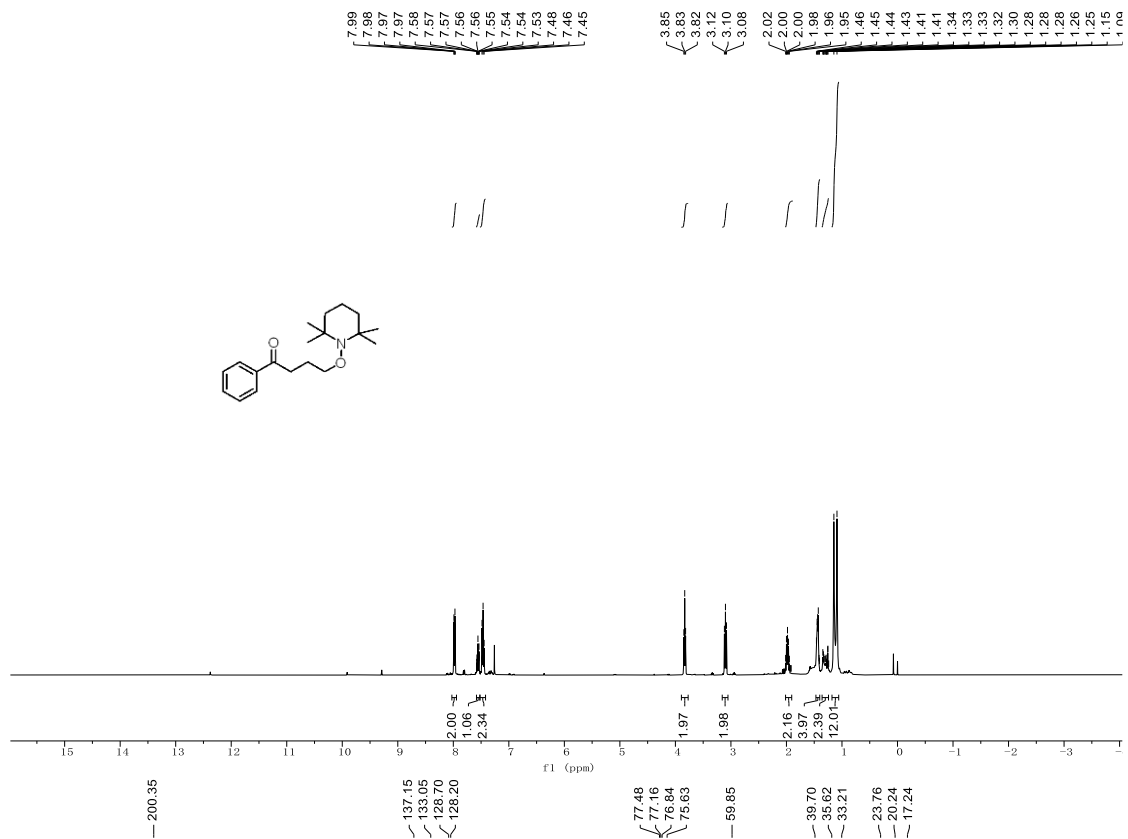
(83) Yang, Q.; Li, Y.; Yang, J.-D.; Liu, Y.; Zhang, L.; Luo, S.; Cheng, J.-P. Holistic Prediction of pK_a in Diverse Solvents Based on Machine Learning Approach. *Angew. Chem., Int. Ed.* **2020**, *59*, 19282–19291.

11. ^1H , ^{13}C NMR spectra of compounds

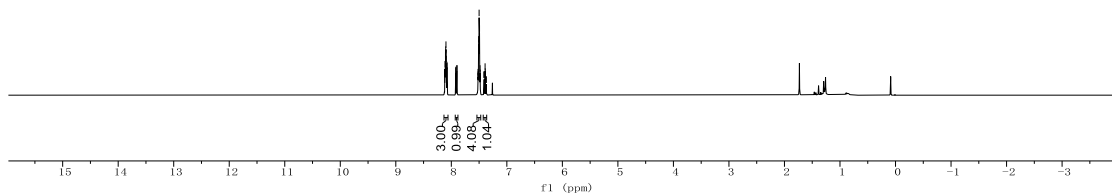
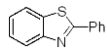




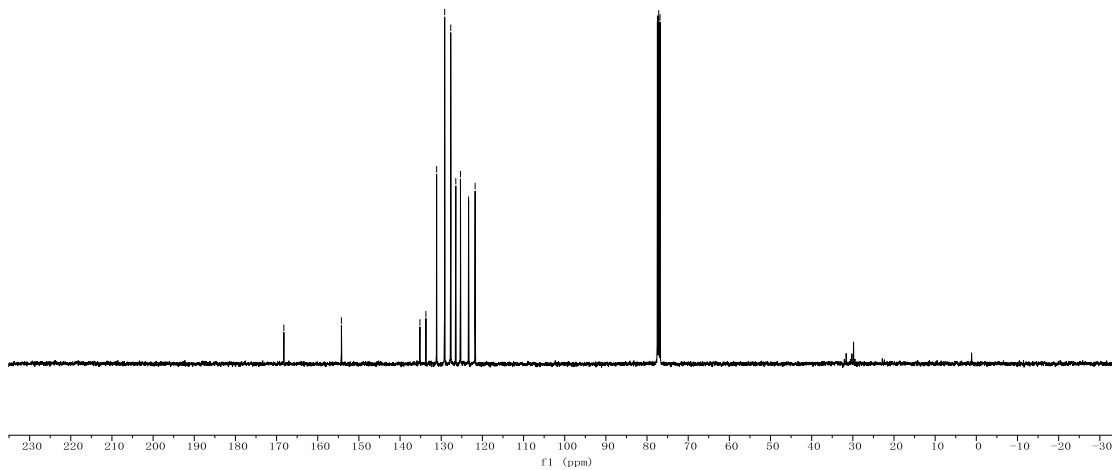
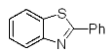




8.12
8.11
8.10
8.09
8.08
8.08
7.92
7.90
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7.52
7.52
7.51
7.50
7.49
7.48
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7.41
7.39
7.37



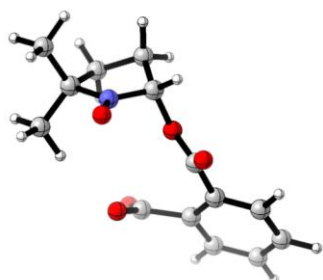
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131.12
129.16
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126.46
125.33
123.35
121.76
77.48
77.16
76.84



12. Cartesian coordinates of optimized structures

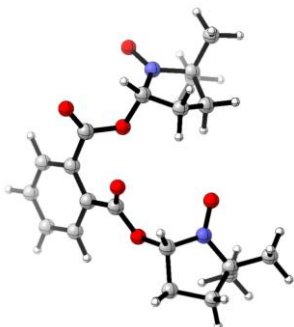
EPR simulation

Adduct-1



C	-10.23925600	-1.54663700	-1.12038300
C	-9.99926100	-1.60041800	0.25931500
C	-10.94812100	-1.09091200	1.15287100
C	-12.14331100	-0.50976700	0.69780400
C	-12.39419000	-0.49189500	-0.69263200
C	-11.43513600	-0.99652100	-1.59096900
C	-13.67102800	-0.00861400	-1.28706800
O	-13.75541800	0.63934600	-2.34237100
O	-14.77303800	-0.49511300	-0.61955400
C	-13.06155100	0.16870600	1.71009000
O	-13.52128900	1.31739600	1.35911500
O	-13.23957900	-0.43553400	2.82552000
C	-16.14137500	-0.20591300	-1.13656000
N	-16.63880000	1.08302500	-0.66597600
C	-17.49137300	1.00259400	0.58051600
C	-17.39281600	-0.51165100	0.90890000
C	-17.06630000	-1.19988000	-0.44167100
O	-16.44467300	2.20750800	-1.30948400
C	-16.89545000	1.91276700	1.66438900
C	-18.92373600	1.43450400	0.21351900
H	-9.50848100	-1.93671400	-1.82189200
H	-9.07636400	-2.03237200	0.63554300
H	-10.76991500	-1.12134000	2.22289700
H	-11.64377800	-0.97327100	-2.65594800
H	-16.10890200	-0.22204800	-2.22478600
H	-16.57929600	-0.68661400	1.62120300
H	-18.32055200	-0.88548700	1.35076200
H	-17.97127100	-1.32721200	-1.04604900
H	-16.58981100	-2.17486700	-0.32196200
H	-16.99973900	2.96544000	1.37497500
H	-17.43022200	1.76542500	2.61045400
H	-15.82958500	1.69667200	1.80788700
H	-19.55232600	1.45156300	1.11089500
H	-18.91160800	2.43979600	-0.22166800
H	-19.37474700	0.74803600	-0.51268400

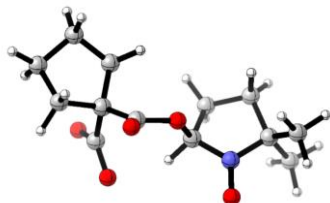
Adduct-2



C	-9.94602900	2.37150500	-0.88881000
C	-9.72107500	1.14660000	-0.25127600
C	-10.70642800	0.15416400	-0.27572400
C	-11.92936300	0.38112600	-0.92751400
C	-12.16737500	1.63252200	-1.54287200
C	-11.16492100	2.61142600	-1.53416300
C	-13.47510800	1.98816000	-2.16799000
O	-13.60879800	2.45136000	-3.30828000
O	-14.50716300	1.82370500	-1.27703700
C	-12.90631700	-0.72494800	-1.08645700
O	-13.68162300	-0.84229400	-2.04813000
O	-12.81547300	-1.65038900	-0.07073700
C	-15.91401600	2.05134000	-1.73619500
N	-16.41997700	3.25060800	-1.08544900
C	-17.34377900	2.99154400	0.08231400
C	-17.22725600	1.45064400	0.21710800
C	-16.79264400	0.93744500	-1.17996500
O	-16.09060800	4.45595000	-1.48012400
C	-16.83591400	3.75734000	1.31107000
C	-18.76049100	3.45136700	-0.31168100
C	-13.68320100	-2.85281600	-0.11041300
N	-14.77129900	-2.69160200	0.85566800
C	-14.76305300	-3.69522800	1.97983700
C	-13.86107300	-4.79548500	1.36588100
C	-12.89379600	-4.05787700	0.40459500
C	-14.14070800	-3.03993800	3.22940100
C	-16.19675800	-4.16094900	2.25390900
O	-15.62641400	-1.70254300	0.78245100
H	-9.18070100	3.14050900	-0.88181100
H	-8.77895700	0.95747700	0.25215000
H	-10.52320000	-0.80744300	0.18789400
H	-11.35172800	3.56804700	-2.01030800
H	-15.89358600	2.17255400	-2.81775300
H	-16.46180200	1.19638800	0.95808500
H	-18.17175400	1.00534800	0.54142500
H	-17.65860500	0.81182500	-1.83957000
H	-16.25245900	-0.00890000	-1.12307800
H	-16.84270300	4.83611600	1.12158100
H	-17.48168600	3.55356400	2.17258500
H	-15.81390400	3.45389200	1.56419400
H	-19.44647200	3.31891000	0.53231400
H	-18.74951700	4.51160100	-0.58827300
H	-19.14131800	2.87448200	-1.16219800
H	-14.08185000	-2.93746400	-1.12191100
H	-13.32198500	-5.35138300	2.13765100
H	-14.48230600	-5.50452700	0.80692200
H	-12.55098900	-4.69503500	-0.41364100

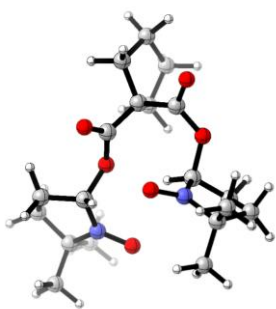
H	-12.01408400	-3.69069100	0.94249000
H	-14.71724600	-2.15348400	3.51734800
H	-14.15034200	-3.74728500	4.06631400
H	-13.10460700	-2.73429000	3.04632900
H	-16.19318500	-4.92826400	3.03595900
H	-16.81776700	-3.32522800	2.59253400
H	-16.64818700	-4.58725800	1.35124700

Adduct-3



C	-16.36005700	0.85920200	1.13662200
C	-15.21202300	1.72585300	0.64308700
O	-15.20132700	2.96339600	0.68837100
O	-14.15045800	1.13529000	-0.05100200
C	-15.87499200	-0.04721800	2.32755900
O	-16.56367800	-1.08651400	2.59377100
O	-14.84048600	0.38365800	2.96758500
C	-13.41326400	-0.10433800	0.33847600
N	-12.00096800	0.17098400	0.09447900
C	-11.44707300	-0.41823500	-1.17916700
C	-12.72503900	-1.04192600	-1.79904200
C	-13.69121300	-1.26920200	-0.60864800
O	-11.27431400	0.90140000	0.90385400
C	-10.83535400	0.70142900	-2.03331900
C	-10.38859900	-1.47340900	-0.80659200
C	-17.53376600	1.74760300	1.68704200
C	-18.81814000	0.99632500	1.29295300
C	-18.49175800	0.47976600	-0.12278700
C	-17.01320700	0.02347000	-0.02686500
H	-13.59054100	-0.27214100	1.40002100
H	-13.17103000	-0.34183600	-2.51443800
H	-12.50081800	-1.97124800	-2.33010600
H	-13.45151300	-2.20398200	-0.08768000
H	-14.73612100	-1.31343300	-0.91580000
H	-10.00282700	1.17660300	-1.50311100
H	-10.45732200	0.29176500	-2.97682400
H	-11.58474400	1.46719300	-2.26207900
H	-9.92906600	-1.88328300	-1.71291100
H	-9.60245900	-1.01904900	-0.19316500
H	-10.83484800	-2.29903500	-0.24020600
H	-17.44112800	1.92213800	2.76489500
H	-17.50066200	2.72524300	1.19345600
H	-19.70777400	1.63680200	1.32458200
H	-18.97956300	0.14967800	1.97120200
H	-19.15496300	-0.32984800	-0.45042500
H	-18.59102100	1.30023000	-0.84727400
H	-16.48378100	0.15642400	-0.97542000
H	-16.96310400	-1.03285700	0.25430500

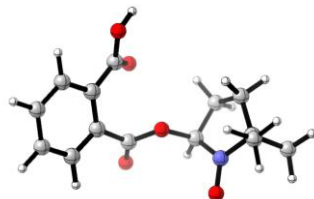
Adduct-4



C	-15.65658600	2.18712000	-0.82686500
C	-14.24330100	2.68457300	-1.25955600
O	-13.97367300	3.87767700	-1.36379700
O	-13.30057400	1.76946900	-1.72248800
C	-15.63160600	1.55675800	0.56334100
O	-15.67124700	2.18328600	1.62297100
O	-15.61463900	0.17338500	0.51520000
C	-12.97869400	0.46082200	-1.09266100
N	-12.15457100	0.69627300	0.08454200
C	-10.68219600	0.45028200	-0.10616600
C	-10.62226000	0.19868600	-1.63729500
C	-12.04157400	-0.28478800	-2.03647800
O	-12.65946100	1.14688600	1.20483700
C	-9.89832400	1.69155500	0.34385900
C	-10.29432100	-0.79073300	0.72430100
C	-15.25922900	-0.55757400	1.77161500
N	-14.91990500	-1.90544900	1.34706900
C	-15.96904300	-2.94693300	1.64703900
C	-17.13149900	-2.05790900	2.16424800
C	-16.45991000	-0.76475100	2.69278700
C	-16.30385700	-3.71212900	0.35871700
C	-15.41283700	-3.89857900	2.72612800
O	-13.82984100	-2.18193100	0.67602400
C	-16.62258200	3.41093400	-0.82593800
C	-17.02393700	3.62055200	-2.31082200
C	-16.67282700	2.29032200	-3.05178600
C	-16.26048900	1.28720400	-1.94813700
H	-13.88926200	-0.06274300	-0.81751800
H	-10.39356800	1.13605600	-2.15528800
H	-9.84945400	-0.53130200	-1.89504200
H	-12.15671000	-1.36019200	-1.86243500
H	-12.28357800	-0.07122100	-3.07957300
H	-8.82334000	1.52879600	0.20635000
H	-10.19909800	2.56956200	-0.23678700
H	-10.09094900	1.89530100	1.40161800
H	-9.22622700	-1.00563600	0.60601500
H	-10.49977000	-0.60526800	1.78363300
H	-10.87226100	-1.66815300	0.41638900
H	-14.40068700	-0.03785700	2.19617700
H	-17.80565700	-1.81360400	1.33559000
H	-17.71661100	-2.56666600	2.93577100
H	-16.09456800	-0.90135900	3.71761700
H	-17.12115000	0.10273600	2.69121200
H	-15.40891300	-4.20914000	-0.02783700
H	-17.06924300	-4.47033500	0.55850000
H	-16.67922100	-3.02904500	-0.41040800
H	-16.12851900	-4.70337400	2.92739700

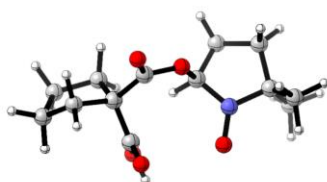
H	-14.47345400	-4.34147800	2.37939300
H	-15.21674600	-3.36605700	3.66356200
H	-17.49694400	3.15491900	-0.21685800
H	-16.14831200	4.28650100	-0.38196200
H	-16.46845400	4.45876700	-2.74184300
H	-18.08994500	3.85893600	-2.39363800
H	-17.50992700	1.90794100	-3.64560500
H	-15.83699500	2.45031800	-3.74366400
H	-15.57050200	0.52003400	-2.30636700
H	-17.13785200	0.77395300	-1.53888800

Adduct-5



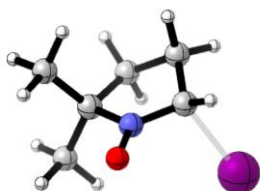
C	-10.12356100	-0.09478300	-1.05979900
C	-9.88559100	-0.83161800	0.10530200
C	-10.92700900	-1.54954300	0.70224600
C	-12.21600600	-1.53392600	0.14491900
C	-12.46216700	-0.76228400	-1.01509700
C	-11.40678000	-0.06365600	-1.61755200
C	-13.81536900	-0.60922000	-1.62295200
O	-14.05073400	-0.70606100	-2.83584600
O	-14.75426800	-0.25220700	-0.68738900
C	-13.26269600	-2.42393300	0.69885500
O	-14.16705700	-2.96064900	0.03928000
O	-13.11573900	-2.65163200	2.04339500
C	-16.18620300	-0.11470800	-1.11329500
N	-16.61609100	1.23515400	-0.79315000
C	-17.47101900	1.34614900	0.44807400
C	-17.38449000	-0.10276300	0.99830800
C	-17.05915100	-0.99546900	-0.22685400
O	-16.27762500	2.26918000	-1.52373700
C	-16.86818400	2.39636500	1.39007800
C	-18.89832300	1.73632500	0.01960600
H	-9.31831200	0.45769600	-1.53225000
H	-8.89335000	-0.85888700	0.54279600
H	-10.73903600	-2.14813200	1.58532900
H	-11.60032900	0.52412700	-2.50818100
H	-13.78870800	-3.29706400	2.36585800
H	-16.22863400	-0.30042100	-2.18480500
H	-16.57683600	-0.16961300	1.73566200
H	-18.31620800	-0.40002100	1.48674200
H	-17.97074700	-1.25461700	-0.77712600
H	-16.54286200	-1.91921200	0.04082700
H	-16.86043900	3.38248600	0.91351800
H	-17.46401200	2.46013600	2.30745200
H	-15.84018700	2.13159200	1.66145800
H	-19.53319000	1.86248900	0.90362100
H	-18.88285300	2.68165400	-0.53428200
H	-19.34363400	0.96596600	-0.62031000

Adduct-6



C	-16.25775200	0.89766900	0.76021800
C	-15.35447600	1.74892500	-0.15162800
O	-15.52591100	2.96058200	-0.31310000
O	-14.31939400	1.17513300	-0.85947200
C	-15.39437400	0.31451300	1.88338600
O	-14.74297400	1.01542500	2.66690700
O	-15.43004600	-1.04902000	1.97367400
C	-13.91740900	-0.26759300	-0.91795100
N	-12.61022700	-0.40577900	-0.30082100
C	-11.45299500	-0.43287800	-1.27138100
C	-12.18628500	-0.17320900	-2.61530200
C	-13.65366500	-0.61585900	-2.37933000
O	-12.45659200	-0.51992600	0.99622700
C	-10.44931200	0.66671100	-0.89824500
C	-10.80128900	-1.82688500	-1.20707500
C	-17.34471900	1.79436600	1.43861900
C	-18.41795500	0.78749700	1.88766700
C	-18.47627100	-0.25851800	0.74081700
C	-17.12287500	-0.14288000	-0.02942800
H	-14.80865800	-1.37254100	2.66880300
H	-14.64940600	-0.88375600	-0.40563100
H	-12.15056300	0.89326700	-2.86103900
H	-11.72070300	-0.72646300	-3.43511900
H	-13.76274200	-1.69854800	-2.50671600
H	-14.36407200	-0.11985300	-3.04377700
H	-9.62291700	0.67725300	-1.61768700
H	-10.92967600	1.65129800	-0.90687800
H	-10.03614500	0.48893400	0.10064800
H	-9.92289700	-1.86020400	-1.86084000
H	-10.47987400	-2.04756200	-0.18322900
H	-11.50164000	-2.60677900	-1.52708300
H	-16.92751600	2.39539100	2.25046700
H	-17.74264400	2.47606500	0.68054700
H	-19.38410500	1.27265200	2.06148300
H	-18.12165200	0.31004200	2.83085900
H	-18.62673900	-1.27102900	1.12914600
H	-19.30966500	-0.04325300	0.06292700
H	-17.29001900	0.24167200	-1.04171900
H	-16.62894600	-1.11065800	-0.12174400

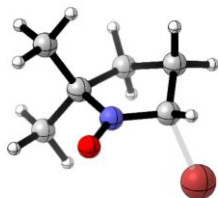
Adduct-7



C	-18.36119100	0.24059400	-0.12128400
C	-17.64602900	1.43555300	0.43386800
N	-16.35365800	1.01569200	0.70348000

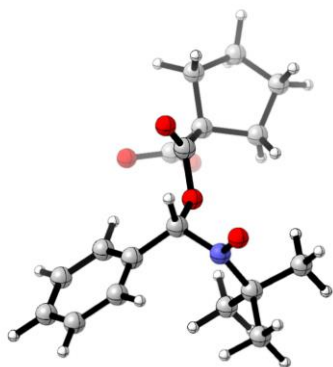
C	-15.97975400	-0.24100600	-0.04300600
C	-17.24903300	-0.50386300	-0.85911600
C	-14.75045500	0.03305500	-0.88800300
C	-15.71441000	-1.31995400	0.99721800
O	-15.53955600	1.62265300	1.44080800
I	-17.58150800	3.10372300	-1.28362500
H	-18.74867900	-0.35263300	0.71174700
H	-19.19690800	0.50458300	-0.75963700
H	-18.07523400	2.03966200	1.21724300
H	-17.14123800	-0.08696200	-1.85786100
H	-17.45098300	-1.56732000	-0.95622800
H	-13.90434600	0.29558100	-0.25804300
H	-14.49352100	-0.85725600	-1.45920900
H	-14.93274000	0.85017600	-1.58178100
H	-15.39140500	-2.23412300	0.50314600
H	-14.93145700	-1.00189100	1.68107000
H	-16.60809400	-1.54316500	1.57781300

Adduct-8



C	-18.35353400	0.26082000	-0.14502000
C	-17.64195000	1.47710200	0.37605100
N	-16.34665100	1.03204600	0.67907700
C	-15.97606500	-0.23409600	-0.04173600
C	-17.24196900	-0.50365400	-0.86256400
C	-14.74208000	0.01925400	-0.88808900
C	-15.71844900	-1.30310900	1.01086300
O	-15.53923600	1.65278100	1.42037600
Br	-17.56909100	2.92703300	-1.15470500
H	-18.73322800	-0.30698100	0.70787000
H	-19.19325800	0.50565500	-0.78588600
H	-18.07758600	2.05240100	1.17904600
H	-17.12426100	-0.10733400	-1.86843100
H	-17.45120100	-1.56722500	-0.94150300
H	-13.89869500	0.29334000	-0.25918000
H	-14.48280200	-0.88207400	-1.44085500
H	-14.91949800	0.82350100	-1.59804900
H	-15.39314900	-2.22389600	0.53048100
H	-14.93970200	-0.97768300	1.69623500
H	-16.61599500	-1.51767900	1.58881900

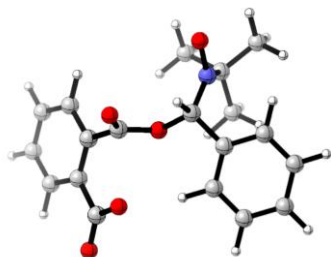
Adduct-9



C	-16.50122200	0.88560400	0.60023700
C	-15.44289700	-0.16830100	0.80409700
O	-15.29112200	-0.90622100	1.78642300
O	-14.57307900	-0.22819600	-0.29082800
C	-17.33768500	0.45911100	-0.67464100
O	-17.74487900	1.37365200	-1.46368100
O	-17.57223500	-0.80405300	-0.76172900
C	-13.46877300	-1.20449200	-0.25511300
N	-12.20041100	-0.49234900	-0.45639000
O	-11.39660600	-0.46182300	0.59955800
C	-17.47209700	0.96481200	1.82266600
C	-17.88360600	2.44721200	1.88892900
C	-16.56783600	3.18830500	1.56927700
C	-15.89522200	2.32670300	0.46753900
H	-13.40317800	-1.58569600	0.76684800
H	-18.31461800	0.27460500	1.70977400
H	-16.93321200	0.68117800	2.73524700
H	-18.30942900	2.72489400	2.86035300
H	-18.63397400	2.66466000	1.11735200
H	-16.72865000	4.22367700	1.24546300
H	-15.93616700	3.22158100	2.46801100
H	-14.80432400	2.32775000	0.56001300
H	-16.16139300	2.69212900	-0.52888300
C	-13.72220600	-2.34680700	-1.22695800
C	-12.66756100	-3.23001900	-1.52002900
C	-14.99717300	-2.58459000	-1.76503100
C	-12.87832200	-4.32875100	-2.36025800
H	-11.68492600	-3.05854800	-1.09091000
C	-15.20132700	-3.68938800	-2.60512600
H	-15.82771100	-1.92431000	-1.52371900
C	-14.14746000	-4.55951500	-2.90977800
H	-12.05577600	-5.00169400	-2.58343400
H	-16.18887100	-3.86761400	-3.02148600
H	-14.31216100	-5.41102900	-3.56339000
C	-11.82090700	0.40482500	-1.62180100
C	-10.39370500	0.00889000	-2.05194300
H	-10.37397700	-1.01915000	-2.43107400
H	-10.05065000	0.67756700	-2.84917000
H	-9.70211000	0.08490300	-1.20811600
C	-11.84334200	1.85953700	-1.10284000
H	-11.48781800	2.53814500	-1.88621100
H	-12.85919600	2.15589600	-0.82107500
H	-11.19176400	1.96171100	-0.22963100
C	-12.79470100	0.24602400	-2.80069700
H	-12.74545100	-0.75419900	-3.23929400

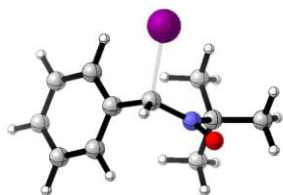
H	-13.82642200	0.45762600	-2.50845700
H	-12.50634700	0.96517800	-3.57579300

Adduct-10



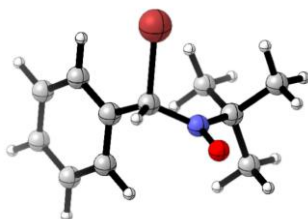
C	-11.96288200	-0.13892500	2.07079400
C	-11.32169300	-1.38234500	2.15862700
C	-11.43025400	-2.29463600	1.10440800
C	-12.17667500	-1.98709200	-0.04250500
C	-12.83188100	-0.74434400	-0.11984600
C	-12.71403100	0.18001800	0.93333900
C	-13.64953500	-0.33417800	-1.30530300
O	-13.32487900	0.53061600	-2.12833300
O	-14.95417200	-0.83756400	-1.22507000
C	-12.23710600	-2.95876300	-1.20730800
O	-12.81737800	-2.50424700	-2.26979400
O	-11.71413300	-4.11426400	-1.05844100
H	-11.87925000	0.57999800	2.87996900
H	-10.73751500	-1.63310300	3.03910400
H	-10.93478800	-3.25892200	1.13982300
H	-13.21140700	1.14306200	0.86499600
C	-15.96259700	-0.29832500	-2.16192600
H	-15.45956300	0.44629000	-2.78390900
C	-16.54733900	-1.40650100	-3.02117000
C	-17.79528900	-1.21615100	-3.64070800
C	-15.81269100	-2.57382800	-3.28570800
C	-18.31607200	-2.19358100	-4.49687200
H	-18.35884400	-0.30726500	-3.45408900
C	-16.34034400	-3.54823500	-4.14514500
H	-14.82793400	-2.70605000	-2.84232600
C	-17.59125300	-3.36664600	-4.74845900
H	-19.28335400	-2.03808400	-4.96549000
H	-15.76844100	-4.45048400	-4.34372500
H	-17.99530700	-4.12631100	-5.41119500
N	-16.94995100	0.48103800	-1.39772000
O	-16.93149100	1.78883000	-1.62604800
C	-17.71523000	0.01964800	-0.16800900
C	-16.98235900	0.58275500	1.07035500
H	-16.88609100	1.67055300	0.99192000
H	-17.55176900	0.34717100	1.97651400
H	-15.98302400	0.14640500	1.16458300
C	-19.13386700	0.61569300	-0.26797500
H	-19.09090000	1.70481500	-0.35164200
H	-19.66231500	0.21718200	-1.14146800
H	-19.70468700	0.35384700	0.62981500
C	-17.79065400	-1.51420100	-0.09532400
H	-18.37386000	-1.93122500	-0.92083500
H	-16.79861700	-1.97311100	-0.09265600
H	-18.29168500	-1.78525800	0.84104400

Adduct-11



C	-13.68032700	0.31086200	-0.86949100
N	-12.51484500	-0.15424800	-0.23000600
O	-12.57346600	-0.27783100	1.03184800
H	-14.46179800	0.25251200	-0.12581600
C	-14.09641900	-0.33988500	-2.15377900
C	-14.52937700	-1.66359200	-2.04745300
C	-14.12852500	0.27588900	-3.39780900
C	-14.95893700	-2.35958200	-3.16517600
H	-14.52263300	-2.15032200	-1.08070400
C	-14.55883500	-0.42109000	-4.51744400
H	-13.82499900	1.30865700	-3.48608100
C	-14.97059700	-1.74046200	-4.40729400
H	-15.29018800	-3.38416600	-3.06305800
H	-14.57630400	0.07492300	-5.47841400
H	-15.30943200	-2.28058900	-5.28118800
C	-11.18364900	-0.45598700	-0.89340800
C	-11.16816900	-1.94692900	-1.22661200
H	-11.87721200	-2.18944000	-2.01267100
H	-10.17316900	-2.22804900	-1.56773800
H	-11.40390900	-2.53812200	-0.34432000
C	-10.09449200	-0.13460000	0.12277500
H	-9.12663800	-0.30325800	-0.34497000
H	-10.14856300	0.90561800	0.43531500
H	-10.16856400	-0.75986500	1.00499400
C	-10.96392900	0.37972200	-2.14479100
H	-11.68088200	0.16104500	-2.92629900
H	-10.99657000	1.44296900	-1.92842900
H	-9.97621500	0.14221400	-2.53515900
I	-13.65188800	2.65796600	-0.98781600

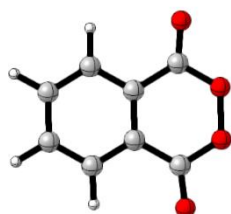
Adduct-12



C	-13.62279600	0.29705600	-0.86644000
N	-12.55826400	-0.42210100	-0.25942100
O	-12.70570100	-0.72341600	0.97063700
H	-14.42301200	0.28909800	-0.13825400
C	-14.08907200	-0.22873400	-2.19374100
C	-14.34771000	-1.59961600	-2.25492100
C	-14.33895600	0.55370400	-3.31223300
C	-14.82311600	-2.17494200	-3.42133800
H	-14.17320700	-2.21574600	-1.38329700
C	-14.81575700	-0.02488300	-4.47994500

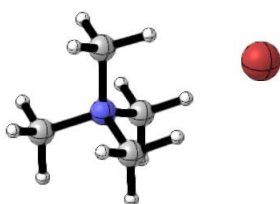
H	-14.14611300	1.61476600	-3.27417600
C	-15.05559500	-1.38869300	-4.54157200
H	-15.01509100	-3.23898900	-3.45315600
H	-14.99862500	0.59787100	-5.34521500
H	-15.42510600	-1.83687900	-5.45417700
C	-11.18375200	-0.63666600	-0.84626600
C	-10.86772400	-2.12123200	-0.69528700
H	-11.53994800	-2.72651600	-1.30049200
H	-9.84965600	-2.30875500	-1.03043500
H	-10.95471500	-2.43045100	0.34168700
C	-10.21599900	0.20372700	-0.01352700
H	-9.19666000	0.01021900	-0.34212000
H	-10.42194700	1.26430900	-0.13171800
H	-10.29691100	-0.05223400	1.03849000
C	-11.09675100	-0.23041300	-2.30810400
H	-11.70349500	-0.85817600	-2.95160000
H	-11.37557100	0.80715900	-2.46291800
H	-10.05958700	-0.34157800	-2.61886600
Br	-13.22016900	2.33911500	-0.88375800

The DFT calculation of potential energy surface PPO



C	-2.69939300	0.70145200	-0.00031500
C	-2.69939200	-0.70145300	0.00040300
C	-1.49646200	-1.40606800	0.00070300
C	-0.28688900	-0.70090400	0.00030900
C	-0.28689000	0.70090600	-0.00046000
C	-1.49646400	1.40606700	-0.00073000
C	0.98178400	1.44940200	-0.00065200
O	2.16269100	0.74228300	0.00120100
O	1.10224500	2.65224200	0.00058300
C	0.98178600	-1.44940100	0.00037700
O	2.16269200	-0.74228400	-0.00109500
O	1.10224400	-2.65224100	-0.00043300
H	-3.64090100	1.24314400	-0.00055200
H	-3.64090000	-1.24314700	0.00073300
H	-1.47282400	-2.49100700	0.00124600
H	-1.47282800	2.49100700	-0.00128100

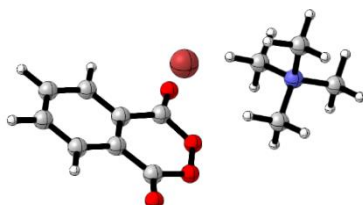
TMAB



N	1.68919300	0.00003900	0.00003200
Br	-2.06402800	0.00000000	0.00000200

C	1.17480900	1.40492000	-0.22489600
H	1.54849700	1.75636200	-1.18924500
H	0.07763200	1.36014700	-0.21751300
H	1.54887900	2.03997500	0.58126100
C	3.18659300	-0.00019100	-0.00014100
H	3.54337200	0.36798400	-0.96454100
H	3.54366200	0.65077000	0.80090800
H	3.54325400	-1.01953400	0.16307600
C	1.17441500	-0.89718700	-1.10410200
H	0.07728700	-0.86835800	-1.06867800
H	1.54805400	-0.51643400	-2.05728600
H	1.54829100	-1.90804000	-0.92657300
C	1.17470400	-0.50755800	1.32914400
H	1.54819500	-1.52349600	1.47569800
H	1.54885500	0.15142300	2.11584600
H	0.07752400	-0.49099000	1.28673200

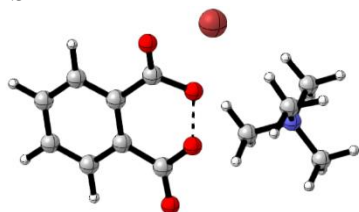
INT1B



C	-3.94119800	0.79506100	-1.32637100
C	-4.31529000	0.66760200	0.01818200
C	-3.50341400	-0.02926100	0.91244700
C	-2.31321900	-0.60089700	0.45643200
C	-1.93810000	-0.47031100	-0.88770300
C	-2.75234000	0.22802100	-1.78287800
C	-0.67178800	-1.03717500	-1.36092400
O	-0.20185600	-0.95901600	-2.47593400
O	0.06999400	-1.81224400	-0.49361900
C	-1.44533200	-1.30163600	1.41181800
O	-1.63237700	-1.44970700	2.59596000
O	-0.30351300	-1.92386700	0.93503500
H	-4.57380700	1.34783900	-2.01506700
H	-5.23697400	1.12244900	0.36986200
H	-3.76385600	-0.12259300	1.96145400
H	-2.43249500	0.33335500	-2.81410900
Br	0.22755000	1.75576700	0.51939200
N	3.49171200	-0.10778300	-0.11319600
C	4.76067700	-0.86094400	-0.36709200
H	4.51168400	-1.87202600	-0.69582400
H	5.33173700	-0.34800300	-1.14409700
H	5.34288900	-0.90274700	0.55611200
C	2.67183100	-0.05017900	-1.38404900
H	2.39667700	-1.06394000	-1.67377700
H	1.77424300	0.53824900	-1.17536300
H	3.27824700	0.42338900	-2.15949200
C	3.80648100	1.29945500	0.33376200
H	2.85536400	1.81286900	0.51390100
H	4.40108700	1.24760600	1.24867800
H	4.37288400	1.79509100	-0.45795500
C	2.69706000	-0.80269300	0.97052300
H	2.45451900	-1.80990500	0.63171600

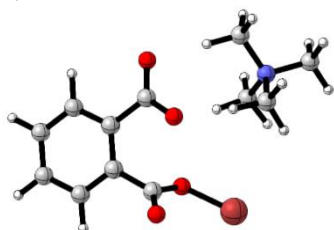
H	3.30954300	-0.83503200	1.87447800
H	1.78183700	-0.22753900	1.13672900

TS1B



C	4.26807000	-0.91016300	1.30379700
C	4.39093800	0.42803900	0.90822400
C	3.43439500	1.00692800	0.07157300
C	2.34421200	0.24747300	-0.36023300
C	2.22639500	-1.09891200	0.02499900
C	3.19100400	-1.67727300	0.85686800
C	1.12938500	-1.93881400	-0.52227300
O	0.96968300	-3.12607000	-0.26955100
O	0.29949200	-1.36314400	-1.40645400
C	1.29138900	0.88543800	-1.19697400
O	1.45059600	1.85500100	-1.89395200
O	0.04374900	0.27625500	-1.06029600
H	5.01751800	-1.35629200	1.95180000
H	5.23130700	1.02187300	1.25728400
H	3.50628500	2.04447400	-0.23854700
H	3.09122200	-2.72392900	1.12721500
Br	-1.03489700	2.28332800	0.46536200
N	-3.17480000	-0.97276400	0.23579200
C	-3.97184200	-2.24023300	0.16288500
H	-4.17834000	-2.59068100	1.17643400
H	-4.90937200	-2.04303700	-0.36137500
H	-3.39122700	-2.98971700	-0.37852500
C	-3.96263900	0.09478400	0.95244300
H	-4.87547600	0.29227600	0.38607700
H	-4.21044900	-0.26697900	1.95283900
H	-3.33922700	0.99217600	1.00716200
C	-2.85792800	-0.49407300	-1.16458100
H	-2.20916400	-1.22793100	-1.64308000
H	-3.80092100	-0.38799300	-1.70575400
H	-2.33727300	0.46128600	-1.08867000
C	-1.89116000	-1.23474500	0.99159500
H	-1.30721300	-0.31184800	0.99511800
H	-2.15341300	-1.53257600	2.00934700
H	-1.35072300	-2.03528500	0.48655400

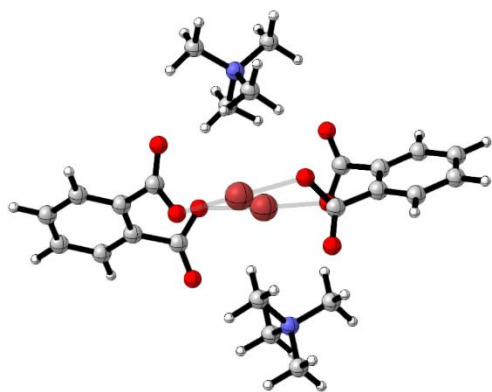
INT2B



C	4.31227000	-1.77350800	-0.55033300
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C	4.65761400	-0.42064600	-0.44844300
C	3.68804900	0.51924700	-0.09488700
C	2.37717300	0.10069100	0.16797600
C	2.02143600	-1.25483400	0.07303300
C	3.00214800	-2.18276600	-0.29333600
C	0.60866800	-1.70839500	0.41094500
O	0.23405300	-2.83618300	0.00408200
O	-0.08615700	-0.86921500	1.06434500
C	1.38299000	1.15907700	0.55645300
O	0.55221500	1.35077900	-0.53505300
O	1.40354000	1.85467400	1.53705100
H	5.06591600	-2.50701200	-0.82652200
H	5.67693900	-0.09775500	-0.64378100
H	3.94344800	1.57236900	-0.01412400
H	2.70986400	-3.22586900	-0.36585300
Br	-0.80189400	2.64268000	-0.28926100
N	-3.22671200	-1.18285700	-0.08211400
C	-4.65693600	-1.09639000	-0.51742800
H	-4.78027100	-1.64904500	-1.45136200
H	-5.29139300	-1.53177200	0.25751200
H	-4.92181200	-0.04765300	-0.66845200
C	-2.85895400	-2.62465800	0.19018600
H	-3.43999700	-2.96681100	1.04970200
H	-3.11576400	-3.21223800	-0.69453700
H	-1.77843000	-2.69283700	0.37507400
C	-3.02453100	-0.36980000	1.17701100
H	-3.23824400	0.67627100	0.94854900
H	-3.71420500	-0.74348300	1.93745600
H	-1.97888400	-0.49319200	1.47677900
C	-2.33173300	-0.63993000	-1.17099000
H	-2.66127600	0.36997700	-1.41989800
H	-1.31329300	-0.61648300	-0.78692500
H	-2.40768800	-1.29722600	-2.03921800

INT2B-d

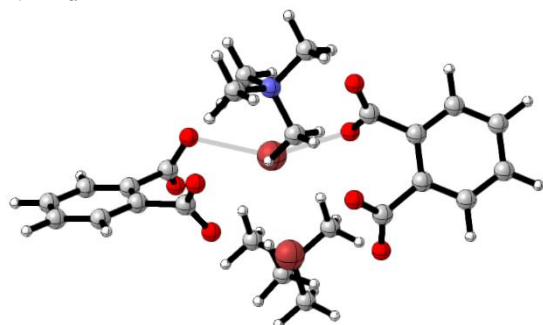


C	-6.53928500	-0.85381600	-0.40388400
C	-6.57747100	0.11179100	0.60668400
C	-5.38635000	0.64518700	1.10728300
C	-4.15331600	0.22253200	0.60187800
C	-4.11579800	-0.73702900	-0.42918000
C	-5.31008500	-1.27467800	-0.91868600
C	-2.80932400	-1.15911800	-1.05900200
O	-2.48236400	-2.33982700	-1.16898200
O	-2.13276500	-0.11452100	-1.47874500

C	-2.87913900	0.75899400	1.21439500
O	-2.14452300	-0.20541000	1.69680200
O	-2.63497300	1.97069400	1.24223000
H	-7.46275300	-1.27455700	-0.79370800
H	-7.53094500	0.44379900	1.00984700
H	-5.40418900	1.38763800	1.90058300
H	-5.26655100	-2.01932600	-1.70877900
Br	-0.09162300	0.15843800	1.90027700
N	-0.32695600	4.08752700	-0.35201200
C	0.69538800	4.93211000	-1.05471900
H	1.05735100	5.69671100	-0.36325400
H	1.51408500	4.28128000	-1.36816500
H	0.22824800	5.40438200	-1.92223900
C	0.32521100	3.39435800	0.82229700
H	1.09942200	2.72480500	0.44911600
H	0.75828500	4.16091600	1.46986600
H	-0.44388300	2.83027700	1.34612900
C	-0.85911500	3.05493900	-1.31876700
H	-1.38006300	3.58035800	-2.12318600
H	-0.01149400	2.49266900	-1.70533100
H	-1.54380100	2.39730900	-0.78487700
C	-1.46666700	4.92613500	0.14853800
H	-1.91797900	5.44988200	-0.69752000
H	-2.19396600	4.26133000	0.61879800
H	-1.08288800	5.64822000	0.87317600
C	6.45876600	0.13246600	0.63987700
C	6.37765500	0.80963600	-0.58082600
C	5.12960100	1.05047900	-1.16224000
C	3.95730000	0.62391400	-0.52974400
C	4.03726800	-0.04140900	0.70989600
C	5.29056300	-0.29078000	1.27936300
C	2.79466400	-0.45237600	1.46937900
O	2.65562600	-1.60596300	1.88954300
O	1.96927500	0.54544600	1.61800200
C	2.63063800	0.83461100	-1.22566300
O	2.04979400	-0.29824600	-1.51104300
O	2.21678400	1.96822000	-1.49360500
H	7.42680000	-0.05999000	1.09569100
H	7.28240400	1.14408000	-1.08237500
H	5.05670500	1.56651900	-2.11599500
H	5.33799500	-0.81169400	2.23179800
Br	-0.07593500	-0.27683500	-1.71490500
N	0.72215200	-4.03473800	-0.14594800
C	-0.00062200	-3.09169000	0.79118200
H	-0.91101300	-3.58071500	1.14112300
H	0.67011300	-2.82905400	1.60861900
H	-0.26567500	-2.19991700	0.23337200
C	1.02110600	-5.31263800	0.57575100
H	1.63839100	-5.08402100	1.44661400
H	0.08134800	-5.76917200	0.89324000
H	1.55605300	-5.98790700	-0.09612100
C	2.01855400	-3.40625800	-0.59905700
H	1.80304700	-2.46993800	-1.11092400
H	2.62836200	-3.18808700	0.27831100
H	2.51911800	-4.10630200	-1.27264100
C	-0.14745100	-4.30761800	-1.34393500
H	-0.36559900	-3.36129000	-1.83790000

H	0.38290700	-4.99373300	-2.00880900
H	-1.08902300	-4.74171200	-1.00529600

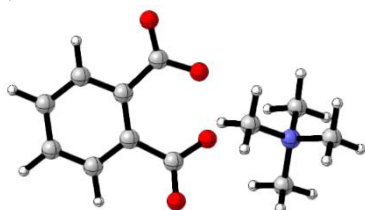
INT4-d



C	-6.80656100	-0.76789700	-0.48393700
C	-6.70831300	-0.00408200	0.68635000
C	-5.45815700	0.41409400	1.14615600
C	-4.29884400	0.08416800	0.43379800
C	-4.39745000	-0.68625300	-0.74023600
C	-5.65395400	-1.10387700	-1.19523800
C	-3.15887300	-1.03819400	-1.53743300
O	-2.87367700	-2.20159600	-1.82009900
O	-2.51349700	0.04856500	-1.84447600
C	-2.96055600	0.53580900	0.99951600
O	-2.22430300	-0.48889600	1.28914800
O	-2.71627800	1.73205800	1.17978800
H	-7.77906200	-1.09848600	-0.83967700
H	-7.60473600	0.26311500	1.24019600
H	-5.37167700	1.00462000	2.05395500
H	-5.71351000	-1.69772300	-2.10300700
Br	-0.12483800	-0.01726900	2.70386900
N	-0.40086500	3.85887600	-0.38035900
C	0.66513800	4.79082300	-0.87970100
H	1.02951800	5.38740400	-0.04018000
H	1.47499200	4.18971200	-1.29739400
H	0.23530200	5.44474800	-1.64256100
C	0.19962200	2.92930300	0.65153100
H	0.99571400	2.35950000	0.18234100
H	0.59641700	3.53923600	1.46655600
H	-0.58678800	2.27338300	1.01788500
C	-0.93558800	3.05290800	-1.54039300
H	-1.39105900	3.74571300	-2.25278600
H	-0.10042000	2.52075400	-1.99513200
H	-1.67584700	2.34564100	-1.16683500
C	-1.52789900	4.62814200	0.24615500
H	-1.95158600	5.30469500	-0.50018700
H	-2.27721100	3.91442700	0.59267200
H	-1.13469300	5.20131300	1.08893000
C	6.50910700	0.45364300	0.70450700
C	6.48023400	1.15090800	-0.50929800
C	5.27172400	1.31792200	-1.18776600
C	4.08434700	0.80008300	-0.65647500
C	4.11200200	0.09961700	0.56615100
C	5.32822900	-0.06460300	1.24011700
C	2.85628400	-0.43402400	1.24384800
O	2.81680000	-1.58120900	1.69764500

O	1.95058400	0.48900100	1.30977500
C	2.79803300	0.94848500	-1.44394700
O	2.32864600	-0.21783300	-1.75094300
O	2.33149000	2.05738600	-1.72889700
H	7.44904000	0.31542700	1.23281500
H	7.39719900	1.55866400	-0.92714700
H	5.23704900	1.85113800	-2.13389600
H	5.33580800	-0.60663800	2.18133600
Br	-0.11090900	-0.27377100	-1.14484800
N	0.50821700	-4.00200100	0.02153300
C	0.01717800	-3.09790500	1.13264300
H	-0.77615200	-3.61847300	1.67267900
H	0.85525200	-2.84652400	1.78207400
H	-0.38077300	-2.18954300	0.68987700
C	0.88506800	-5.33032000	0.60221000
H	1.65837700	-5.17495600	1.35705900
H	0.00245100	-5.78262600	1.05921600
H	1.26313800	-5.97546000	-0.19407000
C	1.72241900	-3.39530800	-0.64377900
H	1.44895100	-2.43142500	-1.06799100
H	2.49724600	-3.24450700	0.10792600
H	2.05393300	-4.07680000	-1.43080600
C	-0.59017500	-4.17248100	-0.99602700
H	-0.85809500	-3.19920600	-1.40885500
H	-0.23662400	-4.84277300	-1.78312800
H	-1.46558200	-4.59587700	-0.50028500

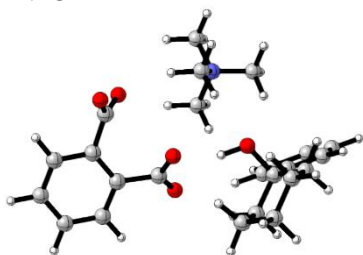
INT4



C	4.08582000	-1.33776600	-0.36289600
C	4.43087400	0.01626100	-0.41864900
C	3.45066400	0.98744400	-0.22285100
C	2.11985700	0.63419300	0.05464700
C	1.77486900	-0.73441900	0.12199500
C	2.76574500	-1.70294800	-0.10454600
C	0.39571500	-1.25862400	0.44774700
O	0.06285700	-2.41279600	0.12062000
O	-0.40643300	-0.48414500	1.10022800
C	1.15312000	1.79286600	0.17815600
O	-0.09690100	1.56421100	0.45254500
O	1.52623900	2.95472900	-0.02797400
H	4.84014400	-2.10475400	-0.52044300
H	5.45644300	0.31488000	-0.62098000
H	3.69368500	2.04305600	-0.28664600
H	2.47376600	-2.74741900	-0.06591700
N	-3.40309700	-0.02067100	-0.22842100
C	-4.79435400	0.21247400	-0.73598300
H	-4.95773700	-0.40104900	-1.62450000
H	-5.50868600	-0.06398100	0.04228600
H	-4.90957200	1.26884400	-0.98716200
C	-3.24020400	-1.47468200	0.15371500

H	-3.94158700	-1.69577400	0.96133000
H	-3.46796300	-2.08711800	-0.72121800
H	-2.21023600	-1.64201100	0.47499500
C	-3.15160300	0.85363600	0.98091200
H	-3.23518000	1.89760000	0.67376900
H	-3.90540200	0.61403900	1.73434200
H	-2.14525100	0.65183800	1.34394300
C	-2.40768400	0.32585200	-1.31018300
H	-2.57508600	1.36002500	-1.61653700
H	-1.40782400	0.22955900	-0.89398800
H	-2.56083900	-0.35475200	-2.15006800

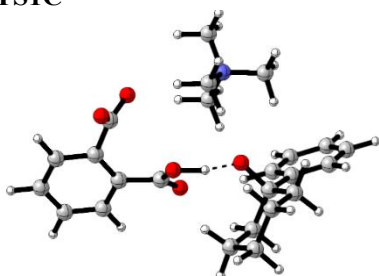
INT5



C	5.90058500	-1.17124900	1.03183700
C	5.00667700	-1.85609600	1.87388400
C	3.63211900	-1.63363700	1.77774900
C	3.11708300	-0.74344600	0.83072000
C	4.02222200	-0.03446200	0.00115300
C	5.41076200	-0.26383900	0.10137000
C	3.56848100	1.02393600	-0.94281800
O	3.02159500	2.08449200	-0.57495700
O	3.84428100	0.83001800	-2.16992400
C	1.61361000	-0.60196700	0.68267800
O	0.92738600	-0.59294800	1.73110100
O	1.18192100	-0.51594300	-0.50630400
H	6.96990000	-1.34552700	1.11318800
H	5.38893800	-2.56555300	2.60353600
H	2.93389800	-2.15033500	2.42915700
H	6.08611100	0.28869700	-0.54546800
C	-3.13162300	-0.34189200	0.70283400
C	-2.38405600	0.12326500	1.80093600
C	-4.45362800	0.10784100	0.57289800
C	-2.93658000	1.01157500	2.72491700
H	-1.35272500	-0.19517900	1.92657500
C	-5.01093600	1.00189200	1.49710600
H	-5.07010500	-0.23090000	-0.25310400
C	-4.25456000	1.46104700	2.57697300
H	-2.33521600	1.34906300	3.56647900
H	-6.03971700	1.33198900	1.37070000
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O	-1.46518900	-0.42512800	-1.01319200
H	-0.53785200	-0.61688100	-0.71146600
N	-0.44397000	2.89585200	-0.84606800
C	0.04827900	4.31084000	-0.89710700
C	0.11618400	2.13813200	-2.03094400
C	0.01499700	2.26540700	0.44904400
C	-1.94722000	2.85182700	-0.89964000
H	-0.29338100	4.77542100	-1.82484000
H	-0.34954100	4.85656000	-0.03867600

H	-0.28589600	1.12839200	-2.01428600
H	1.20131700	2.11754900	-1.94477100
H	-0.33855100	1.24147300	0.47738800
H	1.10289200	2.28309300	0.47648700
H	-2.27910700	3.32509200	-1.82684100
H	-2.34867800	3.38579500	-0.03584600
H	1.13944800	4.29549700	-0.86239900
H	-0.19645900	2.66285500	-2.93744500
H	-2.25102800	1.80455900	-0.86903600
H	-0.41652200	2.83726900	1.27323200
C	-2.44316200	-1.24377700	-0.33915900
C	-1.76758000	-2.45600900	0.34736300
C	-3.40370500	-1.74690300	-1.43556300
C	-1.08203100	-3.40312600	-0.65061200
H	-2.54577700	-3.00014600	0.90151200
H	-1.03565500	-2.10351000	1.08088100
C	-2.70217500	-2.67367100	-2.43948600
H	-4.23867000	-2.28429200	-0.96380500
H	-3.82533300	-0.88391400	-1.96638200
C	-2.05601900	-3.87626800	-1.73772000
H	-0.66755600	-4.26012400	-0.10320800
H	-0.23132600	-2.88869800	-1.11595400
H	-3.42680000	-3.01056000	-3.19301200
H	-1.92806700	-2.10131300	-2.96630300
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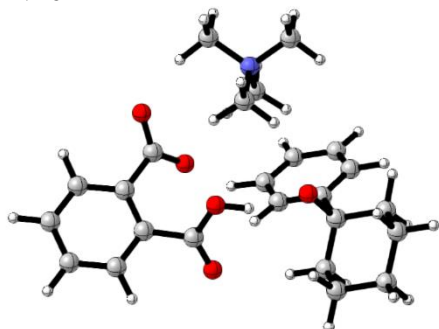
TS1C



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C	-5.05846000	-1.61940600	-1.95844300
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C	-3.09728400	-0.67346500	-0.87874400
C	-3.94123800	0.03163700	0.00977400
C	-5.33671700	-0.12167100	-0.08330300
C	-3.42961500	1.03500400	0.99454200
O	-2.82408500	2.06752200	0.61141200
O	-3.69567400	0.85375200	2.21816200
C	-1.59326300	-0.64195300	-0.78400900
O	-0.89218800	-0.68850500	-1.79683800
O	-1.15183200	-0.60360700	0.44609300
H	-6.97292000	-1.05580100	-1.12541700
H	-5.48692800	-2.25694000	-2.72736300
H	-3.01137500	-1.99528000	-2.55731400
H	-5.97209600	0.42031300	0.61113900
C	3.10539800	-0.45105200	-0.66121100
C	2.46327700	-0.01461300	-1.83688100
C	4.44073200	-0.07174400	-0.46183700
C	3.13310600	0.77233100	-2.77401500

H	1.42561300	-0.28686900	-2.00869500
C	5.11494900	0.72242300	-1.39905800
H	4.97539700	-0.38932700	0.42737900
C	4.46452400	1.15086600	-2.55852800
H	2.61499900	1.08840600	-3.67695700
H	6.15162700	0.99970800	-1.22079400
H	4.98854200	1.76302500	-3.28875400
O	1.24582300	-0.38657500	0.79491800
H	-0.02421100	-0.60899300	0.53913500
N	0.55986900	2.91746700	0.77375000
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C	0.05265600	2.15625900	1.98208200
C	0.08802600	2.26397800	-0.50640400
C	2.06325400	2.90811800	0.78742100
H	0.38236000	4.79925300	1.74316200
H	0.39352800	4.86983000	-0.04449700
H	0.48300500	1.15582600	1.95175700
H	-1.03471200	2.11505500	1.92932300
H	0.49726400	1.25861500	-0.53701300
H	-1.00046900	2.23658900	-0.49866700
H	2.41085200	3.38446000	1.70719400
H	2.43032900	3.45472100	-0.08386900
H	-1.05936100	4.27196700	0.81894800
H	0.38099700	2.69666900	2.87378800
H	2.39020400	1.86800000	0.74177400
H	0.46746000	2.85427200	-1.34360000
C	2.27077900	-1.24357300	0.36551000
C	1.70875200	-2.54180800	-0.28180000
C	3.09960600	-1.64226700	1.62277800
C	0.90585400	-3.39924200	0.70860600
H	2.55606800	-3.12292400	-0.67416100
H	1.07763300	-2.27028000	-1.13358200
C	2.27235600	-2.46965100	2.61432200
H	3.97471500	-2.22594800	1.30129600
H	3.46496200	-0.72806500	2.10679700
C	1.72871300	-3.74598000	1.95652100
H	0.57019500	-4.31507000	0.20334900
H	0.00033700	-2.85833600	1.00980900
H	2.89164500	-2.72096100	3.48629700
H	1.43419000	-1.85948100	2.97503100
H	1.11951200	-4.31470800	2.67151200
H	2.57278300	-4.39401200	1.67119100

INT6

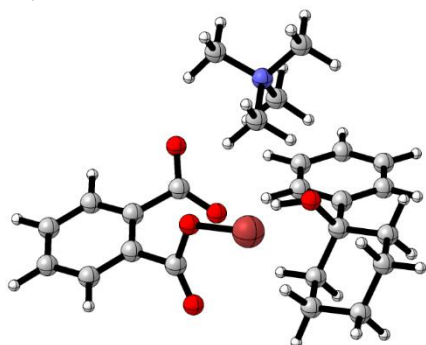


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C	3.74073600	-2.82240600	0.06383900

C	2.96951400	-1.65283900	0.06049400
C	3.58814800	-0.39073600	0.13555300
C	4.98635600	-0.33000800	0.16608300
C	2.77937500	0.89378700	0.26961400
O	1.75482400	0.83957800	1.00773300
O	3.19818300	1.89800100	-0.37312500
C	1.48773200	-1.80407600	-0.03603400
O	0.83259100	-2.56648700	0.65935800
O	0.93868200	-1.07154000	-1.02491800
H	6.84186300	-1.42786300	0.19492400
H	5.72756000	-3.65766700	0.11127300
H	3.23911300	-3.78544500	0.02191600
H	5.45520900	0.64889200	0.20333700
C	-2.44502100	0.08486200	1.11190700
C	-1.18754900	0.02968300	1.74463400
C	-3.33971400	1.11571500	1.45901800
C	-0.84934200	0.95305300	2.73487500
H	-0.45723600	-0.71693100	1.46333100
C	-3.00796500	2.01971800	2.46794400
H	-4.30786800	1.19419000	0.97769900
C	-1.75994600	1.94425100	3.10540000
H	0.14400700	0.90846900	3.16894800
H	-3.72328600	2.78552600	2.75826300
H	-1.50025700	2.66444500	3.87738500
O	-1.80978700	-0.52392900	-0.91902000
H	-0.04603300	-1.09065800	-0.93896800
N	0.07512800	3.23922000	-1.32308700
C	1.34947700	4.04018300	-1.43149400
C	0.26511100	1.90560500	-2.00564100
C	-0.23850700	3.00198400	0.13630100
C	-1.05639200	3.97476900	-1.96937300
H	1.56921100	4.19466500	-2.49089400
H	1.19217100	5.00190900	-0.93694900
H	-0.64238500	1.31548500	-1.87264900
H	1.11100400	1.40022600	-1.54551000
H	-1.19341900	2.47913900	0.19860400
H	0.55738000	2.37987700	0.56872800
H	-0.81373400	4.15587200	-3.01901000
H	-1.20353800	4.92567700	-1.45255700
H	2.14763300	3.45836700	-0.94921100
H	0.45875300	2.08716900	-3.06549800
H	-1.96095000	3.36734800	-1.89539800
H	-0.30834400	3.97338500	0.63146800
C	-2.76850000	-0.95213100	0.00592400
C	-2.53317500	-2.40580800	0.47012800
C	-4.17777300	-0.80478400	-0.60675400
C	-2.74027100	-3.39477800	-0.68707600
H	-3.24282700	-2.61899800	1.28220000
H	-1.52287900	-2.51257700	0.86873300
C	-4.37859300	-1.80090000	-1.76175800
H	-4.92735900	-0.98542000	0.17624500
H	-4.31211800	0.21887100	-0.97437000
C	-4.13386700	-3.24869600	-1.31296500
H	-2.58062400	-4.41772300	-0.32528400
H	-1.97122200	-3.21079100	-1.45155900
H	-5.39100100	-1.68748900	-2.17038600
H	-3.67802700	-1.54726900	-2.57059100

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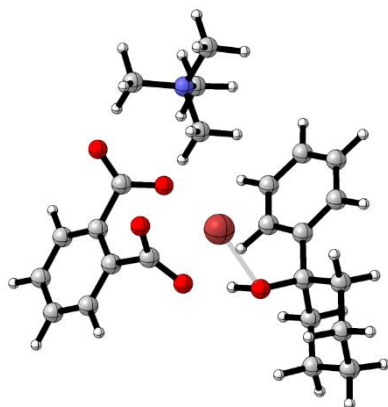
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C	3.48569100	-0.16692400	-0.99912400
C	2.84337100	-1.41747800	-1.02866900
C	3.54702800	-2.52242300	-1.51918800
C	1.39175100	-1.56185000	-0.60440900
O	0.66747900	-0.53821700	-0.78739200
O	1.03396300	-2.66206900	-0.10589500
C	2.81724200	1.05914300	-0.45240100
O	2.67530700	2.11532100	-1.01171800
O	2.52744600	0.81797700	0.87337200
H	5.38324100	-3.25056100	-2.38278400
H	6.49418200	-1.02006700	-2.34517200
H	5.27150400	0.95280000	-1.44182000
H	3.04480000	-3.48503700	-1.52856600
C	-3.25388100	-0.11201000	-1.15482900
C	-2.58474300	-1.25545200	-1.63203700
C	-4.65355100	-0.14941700	-1.09316900
C	-3.28992900	-2.39332200	-2.02432800
H	-1.49867900	-1.26134600	-1.67515700
C	-5.36606500	-1.29015400	-1.48793400
H	-5.20973900	0.71087400	-0.73508100
C	-4.68859300	-2.41776400	-1.95424800
H	-2.74509500	-3.26215200	-2.38704900
H	-6.45236300	-1.29047900	-1.43067000
H	-5.23998500	-3.30253400	-2.26362200
O	-1.50057900	0.65476400	0.31735300
H	-0.72640000	0.19888500	-0.09845400
N	-0.87622600	-2.11877000	2.64124500
C	-1.79168300	-2.01341700	3.82122100
C	0.05313900	-3.29235700	2.80463000
C	-1.69530400	-2.30798300	1.38055000
C	-0.06106800	-0.85005000	2.53196800
H	-1.19694000	-1.86905400	4.72617800
H	-2.45701200	-1.16098500	3.67159800
H	0.69129600	-3.33698000	1.91866700
H	-0.54697000	-4.20124400	2.89134500
H	-0.99369300	-2.43592200	0.55399300
H	-2.31851100	-3.19604900	1.51031400
H	0.51318700	-0.72905600	3.45301600
H	-0.73628400	-0.01097900	2.36991400

H	-2.37721000	-2.93174400	3.90239000
H	0.64522900	-3.14600100	3.71127700
H	0.60260500	-0.94064700	1.67629400
H	-2.29824900	-1.41550600	1.22133900
C	-2.41295600	1.09497600	-0.70432300
C	-1.63440100	1.67516100	-1.91239300
C	-3.24102700	2.21415100	-0.04725100
C	-0.76909200	2.88360600	-1.52888200
H	-2.36970000	1.96109400	-2.67879000
H	-1.00351600	0.89276100	-2.34781800
C	-2.36331400	3.40624200	0.36480400
H	-4.00519000	2.56177600	-0.75558800
H	-3.76571100	1.80656400	0.82737400
C	-1.59819000	3.97605400	-0.83944700
H	-0.28013900	3.28063400	-2.42761800
H	0.03453100	2.55477900	-0.86319700
H	-2.99165700	4.18189300	0.82389200
H	-1.64675100	3.07220100	1.12558600
H	-0.94833400	4.80223100	-0.52113200
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Br	1.57610400	2.18567300	1.75348600

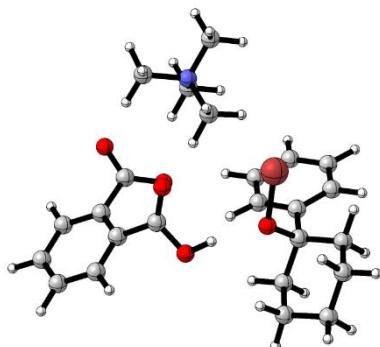
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C	-2.26675400	2.45104600	-0.06990200
C	-3.37144700	1.80449500	0.53522600
C	-4.46401600	2.57673000	0.95473200
C	-3.38523700	0.31148600	0.78328800
O	-2.32429400	-0.18599400	1.26189400
O	-4.43921000	-0.31706300	0.50687200
C	-1.07379500	1.68343000	-0.57258800
O	0.06421900	1.95674400	-0.11192800
O	-1.38736400	0.86816900	-1.50000100
H	-5.32552500	4.54464800	1.09766200
H	-3.38144100	5.67283800	0.01815100
H	-1.43778100	4.31886500	-0.75072000
H	-5.31105600	2.06997500	1.40715800
C	2.33824200	-0.86205400	1.05470100
C	1.07969500	-0.55724500	1.60349400
C	2.80242400	-2.18377000	1.15504100
C	0.32310800	-1.53134700	2.25526500
H	0.65761200	0.43797600	1.51017300

C	2.04838000	-3.16278600	1.81016800
H	3.75844700	-2.46761500	0.73026000
C	0.81223700	-2.83618300	2.37460300
H	-0.65504800	-1.25838200	2.63693000
H	2.43712900	-4.17575700	1.88645300
H	0.23915200	-3.59162700	2.90864400
O	2.47460100	0.95964000	-0.61338200
H	1.57285700	1.34011300	-0.33300400
N	-2.36498400	-3.24556100	-0.56132100
C	-2.02545300	-4.61272100	-1.06866500
C	-3.60363200	-2.73419000	-1.25666400
C	-2.61879100	-3.29735000	0.92498500
C	-1.21017000	-2.30901200	-0.84291700
H	-1.87676800	-4.56357000	-2.14954800
H	-1.10749300	-4.95232900	-0.58452200
H	-3.90369500	-1.79005000	-0.79020400
H	-4.39722700	-3.47546600	-1.13331100
H	-2.77794500	-2.27294300	1.27506400
H	-3.49990100	-3.91828000	1.10231300
H	-1.04317800	-2.29352800	-1.92027400
H	-0.32426000	-2.67857800	-0.32562600
H	-2.84568800	-5.29548800	-0.83582400
H	-3.37305000	-2.60032000	-2.31562700
H	-1.46333400	-1.31500300	-0.47816600
H	-1.73888500	-3.73067700	1.40298900
C	3.18673900	0.24570700	0.42320700
C	3.54145900	1.31564300	1.50632000
C	4.47071500	-0.24839200	-0.26211000
C	4.40980600	2.45405000	0.95350300
H	4.06966000	0.78374800	2.30968200
H	2.61392200	1.70789300	1.93708100
C	5.30999600	0.90426800	-0.83330500
H	5.07342700	-0.79355200	0.47461700
H	4.19430800	-0.95501700	-1.05508900
C	5.67179800	1.91993400	0.26052000
H	4.67965400	3.12747500	1.77731800
H	3.82051200	3.04148700	0.23858400
H	6.21939700	0.49353300	-1.29039600
H	4.74621100	1.40317700	-1.63054400
H	6.24984800	2.74958500	-0.16607500
H	6.31887700	1.43413600	1.00801200
Br	1.09241700	-0.19675900	-2.12657800

INT8



C	5.01298700	-3.45001000	0.60672100
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C	2.81611000	-3.63750400	-0.38260900
C	2.61418600	-2.26374000	-0.19537900
C	3.60442100	-1.47466900	0.41781400
C	4.80627400	-2.08163700	0.79880100
C	3.36749600	-0.00560300	0.74366400
O	2.20516200	0.29990600	1.14515600
O	4.33643000	0.78492200	0.58611900
C	1.37111000	-1.63798200	-0.73796700
O	0.24844200	-2.25760800	-0.31526700
O	1.34610900	-0.70749100	-1.52652000
H	5.94938200	-3.90631400	0.91934300
H	4.16763600	-5.29847200	-0.13234000
H	2.03714400	-4.23261100	-0.85148700
H	5.57138800	-1.45903100	1.25312200
C	-2.28670300	0.63172300	1.29387700
C	-0.91625000	0.61406100	1.60271400
C	-3.05476400	1.72484000	1.72323500
C	-0.33307600	1.64490600	2.34035600
H	-0.27317400	-0.19105000	1.26407100
C	-2.47226200	2.76363900	2.45718600
H	-4.11390000	1.77968900	1.49522200
C	-1.11088300	2.72339500	2.77378600
H	0.73046400	1.58354300	2.54786800
H	-3.08692300	3.59866100	2.78522100
H	-0.66320000	3.52325500	3.36005800
O	-2.09282200	-0.78494600	-0.69503600
H	-0.52741000	-1.75994600	-0.66379900
N	2.03185700	3.29524700	-0.77668700
C	1.57817700	4.58267500	-1.39030200
C	3.25848800	2.79134500	-1.49987700
C	2.37001500	3.50672300	0.67961000
C	0.92416500	2.27141500	-0.88376500
H	1.34310500	4.40937100	-2.44286100
H	0.68723800	4.93270100	-0.86465300
H	3.64792400	1.92072000	-0.96382000
H	4.00779000	3.58689400	-1.49550300
H	2.69109100	2.54642200	1.09216400
H	3.17258200	4.24526000	0.74265700
H	0.74006000	2.06633700	-1.93841500
H	0.03149800	2.67800200	-0.40664200
H	2.37628900	5.32348000	-1.30431800
H	2.97522700	2.54048000	-2.52401000
H	1.24447700	1.36503400	-0.36995300
H	1.47251300	3.86677300	1.18693600
C	-2.88537200	-0.53788200	0.51967100
C	-2.68206900	-1.87365200	1.28967800
C	-4.36848000	-0.38407400	0.14516100
C	-3.24599500	-3.09608200	0.54930900
H	-3.19616400	-1.74341100	2.25169400
H	-1.62098500	-2.01309100	1.51276700
C	-4.89851700	-1.59306300	-0.63871400
H	-4.94070700	-0.27717600	1.07588800
H	-4.51464200	0.53884300	-0.42727500
C	-4.71616800	-2.89414800	0.15614100
H	-3.13630000	-3.97938600	1.19091600
H	-2.64751700	-3.28478700	-0.35026400
H	-5.95803100	-1.43238800	-0.87518100

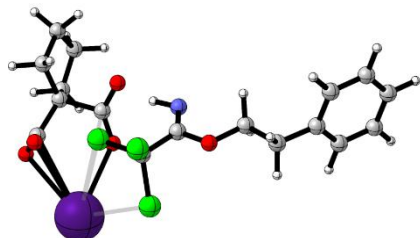
H	-4.36542400	-1.66559300	-1.59530600
H	-5.07489900	-3.75164600	-0.42730200
H	-5.33379400	-2.84970500	1.06685400
Br	-2.07332100	0.60122200	-1.95869100

1-phenylcyclohexanol



C	-0.98396500	0.02258600	0.06771900
C	-1.76126500	-1.14711300	0.15401500
C	-1.65093700	1.22797300	-0.19292400
C	-3.14766600	-1.11575600	-0.00502000
H	-1.28395400	-2.10758800	0.33872900
C	-3.03994200	1.26540500	-0.35967000
H	-1.09566700	2.15626800	-0.26725800
C	-3.79583000	0.09569100	-0.26478800
H	-3.71971700	-2.03743700	0.06848400
H	-3.52891000	2.21547400	-0.56100900
H	-4.87479700	0.12532100	-0.39265600
O	0.80427000	-0.52047000	1.63240200
H	0.20164300	-1.24764100	1.85084400
C	0.53491900	-0.06903700	0.28106200
C	1.16457800	-1.05857500	-0.73317100
C	1.25317300	1.28841700	0.17811600
C	2.68610100	-1.18550300	-0.56478600
H	0.92554500	-0.70597800	-1.74697300
H	0.69505000	-2.04444800	-0.62792300
C	2.77348000	1.16036700	0.36169100
H	1.04808500	1.71984000	-0.81103900
H	0.83944700	1.96775800	0.93214800
C	3.37658100	0.18233600	-0.65660900
H	3.08205200	-1.87016800	-1.32640600
H	2.89905600	-1.63290400	0.41467400
H	3.23413000	2.15188900	0.26135500
H	2.98337700	0.80797800	1.37899500
H	4.45693700	0.07644400	-0.49233700
H	3.24819000	0.58820300	-1.67265100

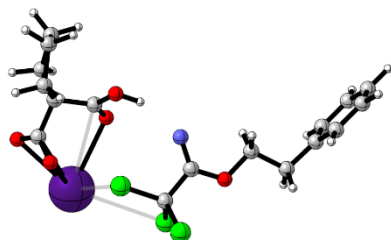
INT9



C	1.67231100	-0.17862200	0.80856400
O	2.91279700	-0.68682500	0.70983000
C	3.93353000	0.18503000	0.17674600
C	5.23361900	-0.61579800	0.16068900
C	0.74154000	-1.28192500	1.38126300

Cl	0.67370400	-2.64634700	0.14748700
Cl	-0.91548700	-0.69170400	1.65899600
Cl	1.41300900	-1.92895300	2.91953800
C	6.37324400	0.21958500	-0.38294000
C	6.65254200	0.24384400	-1.75729000
C	7.67605100	1.04771500	-2.26707100
C	8.43774200	1.84307300	-1.40533200
C	8.16882500	1.82771400	-0.03313200
C	7.14415500	1.02196600	0.47117500
H	3.63889800	0.51008200	-0.82691200
H	4.00909900	1.07585500	0.80929100
H	5.45322900	-0.95166100	1.18109300
H	5.08731500	-1.51415000	-0.45089100
H	6.06500300	-0.37522600	-2.43277600
H	7.87982600	1.05077600	-3.33500100
H	9.23549100	2.46747000	-1.79931000
H	8.75770300	2.44037100	0.64495700
H	6.94162700	1.01217200	1.54050700
N	1.37804100	0.99944500	0.46495400
O	-5.19635000	0.33230700	-0.66994400
C	-4.31387900	0.53078400	0.19371600
C	-3.71028100	2.01090800	0.09373100
O	-3.83316100	-0.21909200	1.06206200
C	-3.82792200	2.73873100	1.43669500
C	-4.30800600	3.00585700	-0.91008500
C	-2.18540200	1.66418300	-0.42830400
C	-3.67529500	4.24946600	1.11803800
H	-4.82898200	2.52729800	1.83701600
H	-3.10712300	2.35765100	2.16251500
C	-3.78140300	4.37279900	-0.43094800
H	-4.06694900	2.76451800	-1.94936500
H	-5.39938500	2.95313100	-0.80891200
O	-2.05735000	0.82231200	-1.32496500
O	-1.38476700	2.39019300	0.18746400
H	-4.45257600	4.83439400	1.62266700
H	-2.70700800	4.61794200	1.46955200
H	-2.79070200	4.55923700	-0.85894100
H	-4.43436700	5.19362200	-0.74750400
H	0.39892600	1.27325000	0.56365500
Cs	-2.91190400	-2.04866900	-1.29613400

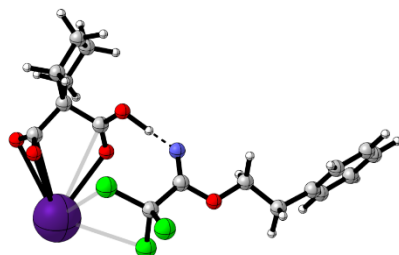
INT10



C	1.67313900	-0.50917500	0.81841700
O	2.90811500	-0.96489200	0.57964200
C	3.89895400	0.02004800	0.17428300
C	5.21345600	-0.72571900	-0.02741300
C	0.69980000	-1.62594200	1.24010000
Cl	0.59272400	-2.80279400	-0.15852300
Cl	-0.91659500	-0.96985700	1.57817400

Cl	1.36670600	-2.47626500	2.67608300
C	6.30831600	0.23389200	-0.44602400
C	6.52972600	0.51951200	-1.80115200
C	7.50910800	1.43879600	-2.18744100
C	8.28188000	2.08758500	-1.21938300
C	8.07001900	1.81034300	0.13471600
C	7.08950700	0.89035700	0.51623800
H	3.55871000	0.50287200	-0.74890000
H	3.97982900	0.78107500	0.95870400
H	5.47724700	-1.23197400	0.90843900
H	5.06521600	-1.50180900	-0.78737500
H	5.93476200	0.01394300	-2.55953400
H	7.67035700	1.64513800	-3.24243200
H	9.04550300	2.80095300	-1.51796400
H	8.66937000	2.30680700	0.89355500
H	6.93268000	0.67500600	1.57153800
N	1.29851300	0.69645800	0.71841800
O	-5.02210200	0.38052200	-0.50232500
C	-4.10728700	0.65216600	0.31510100
C	-3.45324500	2.06933000	0.25409700
O	-3.57810000	-0.15269000	1.14188900
C	-3.65479100	2.86512400	1.56437000
C	-4.05534300	3.01930100	-0.80566300
C	-1.99597100	1.79121500	-0.09499400
C	-3.48851700	4.36101300	1.18447700
H	-4.67773900	2.67135300	1.90906000
H	-2.97857000	2.53625300	2.35588000
C	-3.58335300	4.42101700	-0.37031400
H	-3.76248000	2.75000100	-1.82528500
H	-5.14463900	2.92261800	-0.74540800
O	-1.65396600	1.08859700	-1.04345700
O	-1.09346400	2.36425200	0.71540200
H	-4.26463300	4.97277800	1.65905800
H	-2.52227900	4.74495900	1.52824700
H	-2.59482400	4.63285700	-0.79840100
H	-4.25692300	5.21090900	-0.72277100
H	-0.20489800	2.00471100	0.49880900
Cs	-3.10619500	-1.79493700	-1.39304200

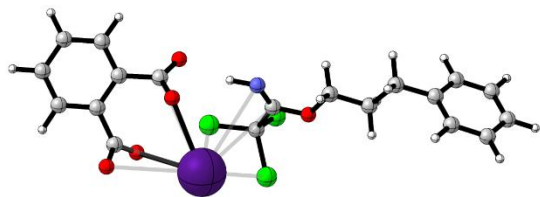
TS3



C	1.49743400	-0.43985100	0.85400900
O	2.74024900	-0.92976600	0.64214700
C	3.74343700	0.01313300	0.19841600
C	5.03752800	-0.77476000	0.01211600
C	0.57497700	-1.62373000	1.27443400
Cl	0.42755600	-2.73193200	-0.18362000
Cl	-1.04442200	-1.09045400	1.76376900
Cl	1.33650000	-2.54288800	2.62305400
C	6.15695900	0.13472900	-0.44916000

C	6.37689800	0.36433700	-1.81526600
C	7.38089500	1.23785900	-2.24254300
C	8.18172300	1.89747500	-1.30502300
C	7.97196600	1.67667800	0.05978000
C	6.96659100	0.80219100	0.48167600
H	3.40965500	0.47812600	-0.73594900
H	3.85180000	0.80143800	0.95141500
H	5.29667100	-1.25591400	0.96260000
H	4.86203700	-1.57347400	-0.71831800
H	5.75903700	-0.14880200	-2.54987600
H	7.53911300	1.40065400	-3.30572900
H	8.96445500	2.57550600	-1.63519600
H	8.59203300	2.18230500	0.79577400
H	6.81048100	0.63178100	1.54524800
N	1.18739600	0.76676600	0.70541800
O	-4.96099600	0.88341300	-0.82078100
C	-4.16099700	0.90656700	0.14867800
C	-3.23991700	2.19618700	0.21310000
O	-3.94600800	0.02552200	1.01106200
C	-3.44037900	2.95351100	1.53950300
C	-3.48679000	3.28999600	-0.84413300
C	-1.82214800	1.58932600	-0.00493300
C	-2.89979500	4.38577400	1.28479800
H	-4.51859500	2.98329700	1.74310600
H	-2.96328100	2.44208100	2.37704100
C	-2.76866400	4.52469000	-0.26233600
H	-3.14042000	2.99931800	-1.84024600
H	-4.56770100	3.45764100	-0.90749400
O	-1.59737100	0.83848800	-0.96150600
O	-0.96332100	1.95209700	0.89081700
H	-3.57750700	5.13926800	1.70205900
H	-1.92690500	4.51807800	1.76833500
H	-1.71080100	4.51123300	-0.55129300
H	-3.19289600	5.46131300	-0.64124800
H	0.07600600	1.37075000	0.78442700
Cs	-3.14013600	-1.74718200	-1.40163000

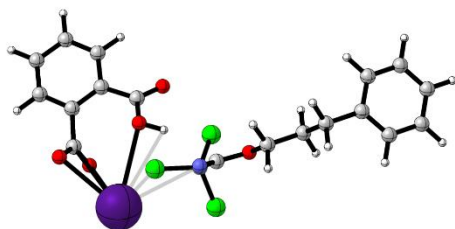
INT11



C	-4.58020100	0.41450300	-0.40019100
C	-5.47991600	0.49680200	-1.64948600
C	-3.12774600	0.70581600	-0.74011000
O	-2.37610300	0.61642900	0.48931000
C	-1.06166200	0.90051200	0.42051300
C	-0.48246400	0.85799300	1.86325600
N	-0.46525500	1.15085800	-0.66292100
H	0.52970100	1.40262000	-0.62159100
C	4.77351800	-0.91861400	0.15709200
O	3.97964000	-0.65454800	1.10168000
O	5.04236200	-2.10014400	-0.18558600
C	3.11618000	1.05555400	-1.30926200

O	2.66840900	-0.07672500	-1.65106000
O	2.40670800	2.05689100	-1.05146400
Cl	-1.26479500	2.12862300	2.86612500
Cl	-0.86145200	-0.78937200	2.58489100
Cl	1.28296100	1.07254400	1.87171300
C	-6.92971500	0.20505900	-1.32682000
C	-7.78670700	1.22778500	-0.89386600
C	-9.11370900	0.95540000	-0.55012200
C	-9.60660700	-0.35067600	-0.63515600
C	-8.76310100	-1.37876400	-1.06716500
C	-7.43663900	-1.09994400	-1.40946100
C	5.40956500	0.21594100	-0.57568900
C	6.81076700	0.33708100	-0.57840600
C	7.41395000	1.42138900	-1.20236300
C	6.62379700	2.40457900	-1.83337300
C	5.23735200	2.29481100	-1.83925700
C	4.61142900	1.20144800	-1.22168100
H	-4.92723500	1.13023200	0.35512000
H	-4.65928500	-0.58347000	0.04915500
H	-5.11826000	-0.21304000	-2.40589000
H	-5.39227300	1.49802200	-2.09261500
H	-2.99259400	1.70791700	-1.16325900
H	-2.71929800	-0.01377000	-1.46003900
H	-7.41092900	2.24728400	-0.82830700
H	-9.76291000	1.76272800	-0.22020000
H	-10.63920300	-0.56423500	-0.37129700
H	-9.13814800	-2.39659300	-1.14200200
H	-6.78697900	-1.90478200	-1.74907300
H	7.40667500	-0.42386300	-0.08303500
H	8.49657000	1.51541000	-1.20304000
H	7.10282400	3.25180100	-2.31712300
H	4.61730500	3.04667000	-2.31788600
Cs	1.59000100	-2.27154000	-0.05724800

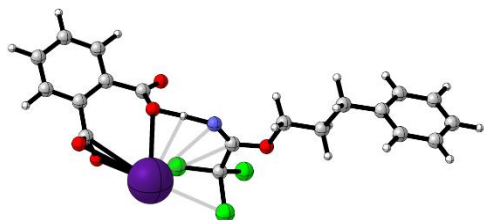
INT12



C	-4.46313800	-0.07453500	-0.20543200
C	-5.32504500	-0.04423300	-1.48394900
C	-3.03035200	-0.47010300	-0.51235900
O	-2.30353100	-0.46467400	0.74827800
C	-0.99672400	-0.70381600	0.69397500
C	-0.30703100	-0.62557700	2.07473500
N	-0.34389200	-1.01460500	-0.35213900
H	0.89612000	0.37274400	-1.17195500
C	4.44854100	0.20469100	-0.39258000
O	3.96063200	-0.39380400	0.61229200
O	4.96672700	-0.33696000	-1.40515500
C	1.84547100	1.85350500	-0.50219200
O	1.81022900	0.71932000	-1.25331000
O	0.81697700	2.32547100	-0.04288400
Cl	-0.86978900	0.81790600	2.96367400

Cl	-0.78711300	-2.13462600	2.96873800
Cl	1.46161000	-0.56355400	1.85290100
C	-6.75562200	0.35562800	-1.19087700
C	-7.13139100	1.70674800	-1.17437200
C	-8.43998500	2.08280500	-0.85890400
C	-9.39573300	1.10831600	-0.55466200
C	-9.03333600	-0.24208800	-0.56956100
C	-7.72303000	-0.61252400	-0.88561900
C	4.39659000	1.72403500	-0.36823000
C	5.60879900	2.42156100	-0.28060600
C	5.63584700	3.81102000	-0.15689900
C	4.43923400	4.53717000	-0.12236200
C	3.22638600	3.86073300	-0.22254200
C	3.19381500	2.46172800	-0.35925200
H	-4.46929700	0.91265400	0.27154100
H	-4.88975900	-0.78265300	0.51524900
H	-5.30662300	-1.03440900	-1.95945200
H	-4.88298900	0.65908600	-2.20258400
H	-2.54368600	0.24102100	-1.19067900
H	-2.96333300	-1.47536100	-0.94665200
H	-6.39353700	2.47058900	-1.41306000
H	-8.71324800	3.13499700	-0.85437000
H	-10.41456300	1.39858700	-0.31171800
H	-9.77047500	-1.00721600	-0.33904900
H	-7.44898400	-1.66601000	-0.89867700
H	6.53519800	1.85468600	-0.30550400
H	6.58967000	4.32851700	-0.08449000
H	4.45330400	5.61935100	-0.02361900
H	2.28512600	4.40197700	-0.20593600
Cs	2.86538600	-2.45976100	-1.19287300

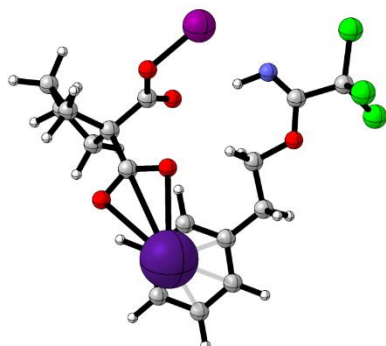
TS4



C	-4.49474400	0.45571100	-0.20380200
C	-5.30937200	1.14452000	-1.31719900
C	-3.00020300	0.57724000	-0.45082200
O	-2.33176800	-0.09020900	0.64121400
C	-0.97823200	-0.03706900	0.64375900
C	-0.47281100	-0.82794900	1.89457700
N	-0.27818600	0.49260500	-0.24923700
H	0.95301500	0.75311900	-0.32278600
C	4.71023800	-0.29150000	-0.51328400
O	4.32106600	-0.87579700	0.53651700
O	4.83509600	-0.89334300	-1.61478200
C	2.64908300	1.87455000	0.19970800
O	2.14344000	0.91762000	-0.54784500
O	2.01679800	2.54844900	1.00496100
Cl	-1.37791500	-0.37436900	3.37216900
Cl	-0.78222800	-2.60905200	1.51927600
Cl	1.26895000	-0.60967600	2.16928600
C	-6.80069200	1.03067600	-1.08474300

C	-7.47765700	1.97684400	-0.30103800
C	-8.84592300	1.85066100	-0.04548600
C	-9.56158600	0.77109900	-0.57303500
C	-8.89867200	-0.17799200	-1.35722400
C	-7.52993000	-0.04639900	-1.60918300
C	5.05318500	1.16054000	-0.43200400
C	6.38841200	1.52765800	-0.69237300
C	6.78692300	2.85561400	-0.59781900
C	5.85276600	3.83910100	-0.23234400
C	4.52874100	3.48585800	0.02721600
C	4.11062800	2.15259100	-0.06542100
H	-4.73936700	0.90429300	0.76675100
H	-4.77108600	-0.60433800	-0.14276700
H	-5.05036600	0.69753500	-2.28678700
H	-5.02210100	2.20321900	-1.37310300
H	-2.66924200	1.62192800	-0.48169900
H	-2.69978100	0.10293700	-1.39388800
H	-6.92770200	2.82130100	0.11042000
H	-9.35304500	2.59650400	0.56165200
H	-10.62634900	0.67262600	-0.37792000
H	-9.44698400	-1.01834100	-1.77600800
H	-7.02117300	-0.78733700	-2.22343600
H	7.09710400	0.75499900	-0.97574000
H	7.81780400	3.13108100	-0.80374500
H	6.16268600	4.87703100	-0.14311600
H	3.79909500	4.23347500	0.32188500
Cs	2.02649300	-2.14745300	-1.22990800

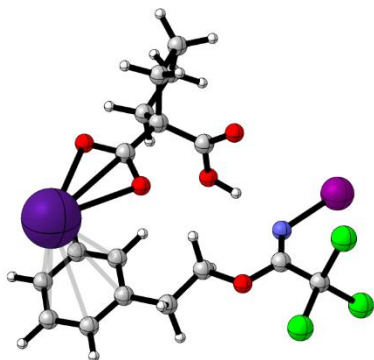
INT13



O	3.65413200	1.18594000	-0.31347500
C	2.39806100	1.25680600	-0.24638600
C	1.82040400	2.39785500	0.64669500
O	1.57078600	0.48185800	-0.81218000
C	2.36175500	3.79223300	0.25774100
C	2.28053200	2.29405000	2.12179900
C	0.28860200	2.27736000	0.56512100
C	2.04293200	4.67666900	1.47906000
H	3.44359900	3.67883500	0.12843800
H	1.94252000	4.17078400	-0.67751000
C	2.11779900	3.72057100	2.70768000
H	1.72178200	1.53945400	2.68111400
H	3.33549500	2.00172600	2.09724700
O	-0.39330000	1.60735700	1.31832000
O	-0.18248900	3.00544700	-0.45990000
H	2.73177400	5.52484000	1.56177200

H	1.03284500	5.09367700	1.38268200
H	1.20519600	3.78979100	3.31024200
H	2.95535000	3.96921300	3.36932100
I	-2.20101700	2.87062200	-0.91094400
Cs	3.65787800	-1.36917600	-1.80321600
C	-3.09063600	-1.08570000	0.58310900
O	-2.05116500	-1.90569100	0.31831700
C	-0.74642000	-1.54205200	0.81287300
C	0.10437400	-2.79565300	0.66099000
C	-4.39108100	-1.77845400	0.11536200
Cl	-4.26365900	-2.10871400	-1.66400600
Cl	-5.83039400	-0.77168200	0.41555800
Cl	-4.57425400	-3.35105900	0.99809900
C	1.52813000	-2.67997200	1.17248500
C	2.04271800	-1.50215700	1.73582600
C	3.37119400	-1.43718000	2.17385200
C	4.20844500	-2.55104100	2.06222500
C	3.70572000	-3.73712600	1.50896900
C	2.37928500	-3.79649000	1.06992400
H	-0.34827900	-0.70027500	0.23782900
H	-0.83254000	-1.24330500	1.86486400
H	-0.40264700	-3.62126000	1.17790400
H	0.11575500	-3.07165000	-0.40264700
H	1.42436200	-0.61470800	1.80490900
H	3.75010100	-0.50457700	2.58138300
H	5.23777100	-2.50000000	2.40834200
H	4.34069700	-4.61704200	1.43265500
H	1.99113600	-4.72373800	0.65064400
N	-3.13035600	0.05854600	1.11363000
H	-2.21520400	0.45725000	1.33565300

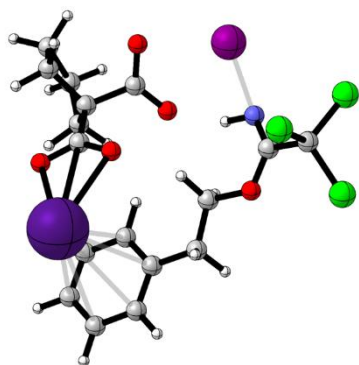
INT14



O	3.68803700	1.77097600	-0.55770800
C	2.44113600	1.57473700	-0.58788600
C	1.53179300	2.78849800	-0.23964600
O	1.87664400	0.47940300	-0.89607100
C	1.65360800	3.90391100	-1.30446400
C	1.97682500	3.53295800	1.04092700
C	0.09334600	2.29269300	-0.14028800
C	1.18391000	5.20018100	-0.59435700
H	2.71085500	3.97567200	-1.58045400
H	1.07185800	3.67318900	-2.20068700
C	1.28941700	4.90992500	0.93391800
H	1.72255700	2.99344100	1.95811100
H	3.06651900	3.63095200	0.98962100

O	-0.15984600	1.66849400	1.03771600
O	-0.75881900	2.41399900	-0.99955900
H	1.80057800	6.05693400	-0.89051500
H	0.15090600	5.43717500	-0.87139100
H	0.28807400	4.86154500	1.38027400
H	1.84210200	5.68690600	1.47504500
I	-4.09337000	1.41581700	0.62558300
Cs	4.42196200	-0.96551100	-1.30872500
C	-2.52363500	-1.13478300	0.06495300
O	-1.44150600	-1.91276500	0.12968200
C	-0.23795900	-1.38815700	0.75125500
C	0.72437700	-2.55803800	0.86459700
C	-3.68105400	-1.89838000	-0.65603600
Cl	-4.19197100	-0.96209900	-2.10217400
Cl	-5.05119200	-2.09994800	0.50028900
Cl	-3.18411800	-3.54016500	-1.20788900
C	2.04707700	-2.20421400	1.52433400
C	2.36472600	-0.90311200	1.94847700
C	3.60782800	-0.62681600	2.53217700
C	4.55482700	-1.64164800	2.70107500
C	4.24884900	-2.94442600	2.28366600
C	3.00615000	-3.21806900	1.70356100
H	0.16755300	-0.59325300	0.12108900
H	-0.50333100	-0.98244500	1.73215900
H	0.24184000	-3.37019300	1.42493900
H	0.91049300	-2.95161500	-0.14422800
H	1.66800300	-0.08591500	1.79642900
H	3.83519500	0.39175000	2.83463700
H	5.51622100	-1.42434700	3.16008500
H	4.96934600	-3.74726000	2.42332500
H	2.76999300	-4.23453700	1.39160200
N	-2.50173600	0.04174000	0.56670400
H	-1.03555200	1.21983700	0.95307600

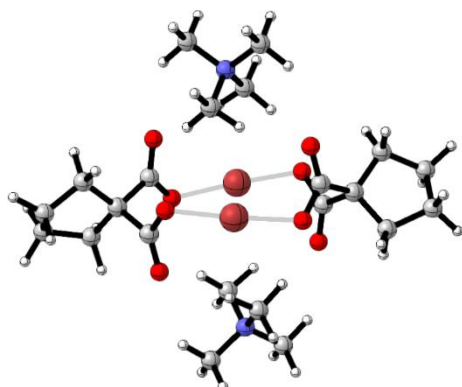
TS5



O	-3.37246300	-1.29590700	-0.70983100
C	-2.11772600	-1.35061300	-0.54597700
C	-1.58747900	-2.64738100	0.13053600
O	-1.30398000	-0.43785200	-0.88941200
C	-2.01771300	-3.90533400	-0.66107100
C	-2.25664000	-2.91342100	1.50247400
C	-0.04679300	-2.54637200	0.33314600
C	-1.93486600	-5.07402900	0.35152100
H	-3.05231700	-3.74802500	-0.98347400
H	-1.39590600	-4.06540600	-1.54549500

C	-2.01085800	-4.41513300	1.76243400
H	-1.85377400	-2.27305400	2.29302100
H	-3.32769700	-2.70764500	1.39041100
O	0.37190200	-1.74080100	1.21247400
O	0.65031300	-3.31665400	-0.40633000
H	-2.74566300	-5.79528200	0.19217700
H	-0.99033900	-5.61475400	0.23245400
H	-1.06103800	-4.54778500	2.29461700
H	-2.79465700	-4.85304300	2.39233400
I	3.08241600	-1.94354600	-0.38020700
Cs	-3.47791100	1.35923200	-1.82715700
C	2.64899700	1.15476700	0.67413100
O	1.63552200	1.97152900	0.88931000
C	0.33302200	1.40693600	1.26493200
C	-0.60845300	2.59533500	1.34491600
C	3.83479800	1.87365000	0.00585000
Cl	3.46039200	1.92743700	-1.76487600
Cl	5.37468200	1.01209900	0.27983200
Cl	3.98950000	3.55003500	0.64142100
C	-2.04889200	2.22353500	1.65128700
C	-2.45566800	0.90363300	1.89863200
C	-3.80468300	0.60542100	2.12707600
C	-4.76409600	1.62099000	2.12473600
C	-4.36775700	2.94557700	1.89245700
C	-3.02158900	3.24055000	1.65795400
H	0.02934200	0.67187500	0.50967200
H	0.44336000	0.90818000	2.23280100
H	-0.23605700	3.30045900	2.10029300
H	-0.56345900	3.12875800	0.38525500
H	-1.74058400	0.08797000	1.87000700
H	-4.09714300	-0.42923300	2.27619400
H	-5.81031000	1.38580100	2.30332000
H	-5.10332100	3.74680900	1.90308700
H	-2.71741700	4.27157300	1.48176400
N	2.66315600	-0.10650300	0.93157700
H	1.78223000	-0.54536700	1.27683600

UV spectrum prediction
BCTC-2d(TMA)

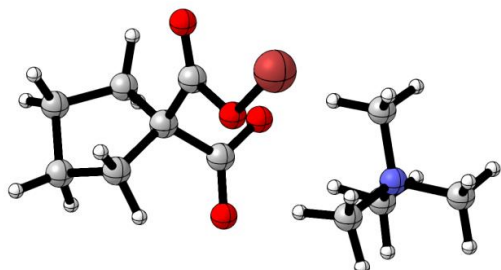


C	2.70116600	-0.62522000	-0.96310400
O	2.13177800	0.29695100	-1.69468700
O	2.46680900	-1.83582200	-1.01641500
Br	0.05601100	0.01897500	-1.99154700
N	0.03869000	4.14604900	-0.00573700

C	-1.07059500	5.00435200	-0.53731600
H	-1.43414700	5.65148000	0.26443700
H	-0.68783500	5.60982900	-1.36234700
H	-1.86785600	4.34470500	-0.88632800
C	1.16327500	4.98219500	0.52886800
H	1.53885600	5.62518600	-0.27066200
H	0.79145200	5.59185000	1.35581400
H	1.94819600	4.30694700	0.87599600
C	0.56016000	3.27270400	-1.12349000
H	-0.27883900	2.70558800	-1.52111000
H	0.99079700	3.92334500	-1.88905900
H	1.31675000	2.59939300	-0.72039100
C	-0.49850600	3.27829200	1.10894600
H	-1.26740100	2.62070800	0.70326600
H	0.33004200	2.69446200	1.50426000
H	-0.91708200	3.93391100	1.87695100
C	3.66439800	-0.01616700	0.11038200
C	4.58278100	-1.09893200	0.75942200
C	4.62788900	1.04021400	-0.49210700
C	6.02967800	-0.59918500	0.55670600
H	4.42243500	-2.05038900	0.24365900
H	4.33065800	-1.26062600	1.81087100
C	5.94346400	0.27715600	-0.70365000
H	4.77228100	1.84283700	0.24094600
H	4.22144500	1.49529300	-1.39807100
H	6.34393500	0.02036000	1.40848400
H	6.74944300	-1.42181400	0.46825900
H	6.80650700	0.94150400	-0.83276500
H	5.87602400	-0.35714900	-1.59934900
C	2.64269000	0.60641100	1.10151200
O	2.00708800	-0.30695000	1.79441900
O	2.42978500	1.82098500	1.13848800
C	-2.71758800	-0.57667800	0.94573800
O	-2.13131500	0.33254400	1.68029100
O	-2.50762700	-1.79164000	0.99779700
Br	-0.06130200	0.01416400	1.97451100
N	-0.03779600	-4.11098500	-0.01226000
C	0.43459800	-3.24608500	1.13343900
H	1.22265800	-2.58452100	0.77354800
H	-0.41629600	-2.66610400	1.48465600
H	0.81242500	-3.90317900	1.92104700
C	-0.49943900	-3.23414700	-1.15339400
H	-1.27780800	-2.56369100	-0.78893400
H	0.35894300	-2.66415700	-1.50259400
H	-0.88690400	-3.88204800	-1.94388900
C	-1.18768700	-4.95203500	0.45663700
H	-0.86009400	-5.56442600	1.30008500
H	-1.99192900	-4.28001800	0.76353800
H	-1.51775100	-5.59229800	-0.36486000
C	1.10136100	-4.96424300	-0.48552000
H	1.42263300	-5.61330500	0.33256700
H	0.76600100	-5.56762800	-1.33240400
H	1.91431400	-4.30093100	-0.78830100
C	-3.66533000	0.05682900	-0.13023100
C	-4.60796100	-1.00302300	-0.78040800
C	-4.60735000	1.11909700	0.48398600
C	-6.04861900	-0.59352200	-0.38399700

H	-4.35020300	-1.99276300	-0.39441200
H	-4.47016500	-1.03873600	-1.86478900
C	-5.86856200	0.32109300	0.84099600
H	-4.83856000	1.87041300	-0.28149300
H	-4.14735900	1.63827200	1.32742500
H	-6.51809300	-0.02125800	-1.19588600
H	-6.69082200	-1.45970800	-0.18524200
H	-6.73939200	0.95811100	1.03737300
H	-5.68902000	-0.28196000	1.74261600
C	-2.63483500	0.66216600	-1.11742800
O	-2.01818100	-0.26161300	-1.81419000
O	-2.40074400	1.87299200	-1.15152600

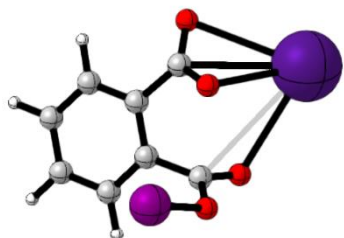
BCTC-2(TMA)



C	-1.29466100	0.83032000	-0.47619100
O	-0.23862900	1.06277200	0.39275200
O	-1.64492400	1.60974600	-1.32215400
Br	0.66216200	2.70370400	0.19105500
N	3.06048400	-1.17254900	-0.00333000
C	4.53676700	-1.00564500	0.18800300
H	4.87032200	-1.66554600	0.99166900
H	5.04967900	-1.26472400	-0.74052000
H	4.74504400	0.03413000	0.44987900
C	2.73693900	-2.61419800	-0.32699000
H	3.31079000	-2.90082700	-1.21149400
H	3.02186200	-3.22942100	0.52900600
H	1.66144200	-2.68135500	-0.52075200
C	2.59939200	-0.29367900	-1.14458100
H	2.79893800	0.74664500	-0.88260900
H	3.16039700	-0.57782600	-2.03796600
H	1.53104100	-0.47321700	-1.29868500
C	2.34421500	-0.78126500	1.26966800
H	2.45913600	0.29402000	1.41601100
H	1.29262700	-1.05923500	1.18555900
H	2.79996300	-1.33165000	2.09592200
C	-1.88962200	-0.52489900	-0.09738700
C	-2.59454200	-0.41220400	1.28991500
C	-3.00675400	-0.94231600	-1.11032600
C	-3.90982800	-1.18785200	1.11595600
H	-2.81725600	0.63779900	1.52370700
H	-1.94655600	-0.81149800	2.07296100
C	-4.32650300	-0.84684700	-0.32364000
H	-2.81950700	-1.97558500	-1.42118400
H	-2.98939300	-0.32366700	-2.00991900
H	-3.71586400	-2.26510400	1.20588800
H	-4.66303900	-0.91792000	1.86587100
H	-5.10116900	-1.51237000	-0.72323600
H	-4.71838900	0.17930800	-0.36340200

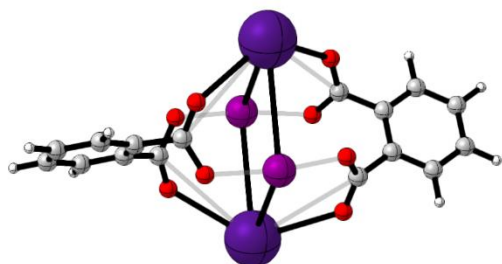
C	-0.71153400	-1.56535300	-0.13887400
O	-0.44435700	-2.22130000	0.89454100
O	-0.10113200	-1.60873200	-1.24809500

BCTC-3



C	1.90330700	3.67147900	-0.11995600
C	2.51548200	3.01309400	0.95278100
C	2.05329200	1.75770900	1.35751000
C	0.99094700	1.15835400	0.67149300
C	0.37624600	1.81028300	-0.40901800
C	0.82849100	3.07678300	-0.78685600
C	-0.76608100	1.10261600	-1.11498100
O	-1.72823200	1.78904900	-1.54096200
O	-0.67770700	-0.16709400	-1.11402800
C	0.41996400	-0.13457100	1.17783000
O	-0.59234000	-0.19987200	1.86007200
H	2.26173000	4.64945100	-0.43178700
H	3.34625300	3.47698500	1.47811900
H	2.51373000	1.24926600	2.20106400
H	0.32685600	3.57924200	-1.60873700
Cs	-3.27688400	-0.47697000	0.11631000
O	1.11300600	-1.29331500	1.05392000
I	2.58362900	-1.51860800	-0.38642500

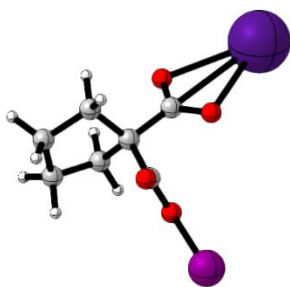
BCTC-3d



C	-6.59911900	0.45593800	0.52720300
C	-6.59847100	-0.46013000	-0.52847600
C	-5.38652500	-0.91154100	-1.05960300
C	-4.17245100	-0.45566600	-0.53828600
C	-4.17311300	0.45301500	0.53863200
C	-5.38782000	0.90814400	1.05911700
C	-2.87492400	0.88555500	1.18239000
O	-2.50218600	2.06593500	1.17787400
O	-2.24907000	-0.12410800	1.71762500
C	-2.87358000	-0.88721400	-1.18150700
O	-2.24879800	0.12288500	-1.71717000
O	-2.49965400	-2.06717700	-1.17646700
H	-7.53870600	0.81316000	0.94092600
H	-7.53755900	-0.81794600	-0.94282000
H	-5.37642100	-1.61438100	-1.88840900

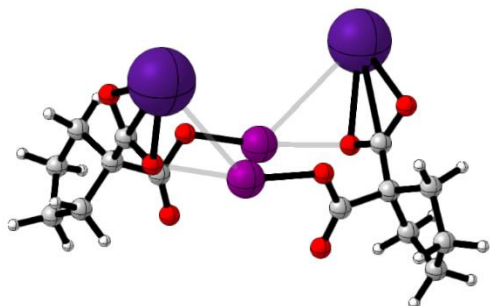
H	-5.37870400	1.61101800	1.88790400
C	6.59915100	0.46024900	-0.52694200
C	6.59928800	-0.45716800	0.52750200
C	5.38768600	-0.90983700	1.05844600
C	4.17325300	-0.45380500	0.53822200
C	4.17313300	0.45630700	-0.53756600
C	5.38741800	0.91257600	-1.05788900
C	2.87446500	0.88886500	-1.18046100
O	2.50032100	2.06871300	-1.17359000
O	2.24994700	-0.12056900	-1.71794200
C	2.87484800	-0.88694200	1.18127300
O	2.24900000	0.12194700	1.71773200
O	2.50214800	-2.06736700	1.17527300
H	7.53838600	0.81849800	-0.94057700
H	7.53863900	-0.81515700	0.94109600
H	5.37823300	-1.61384100	1.88627100
H	5.37782700	1.61643000	-1.88584600
I	0.00048900	0.00179900	-2.03232400
I	-0.00029900	-0.00153500	2.03260400
Cs	0.00163100	-3.42721200	-0.00147600
Cs	-0.00244700	3.42714100	0.00052400

BCTC-4



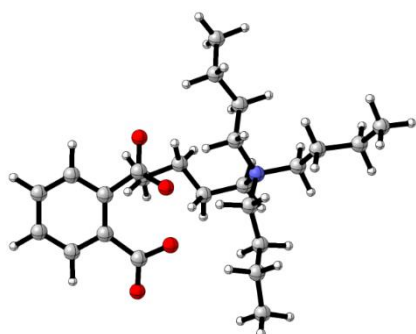
O	2.00250300	1.42530600	-0.53416500
C	1.01260200	0.84491100	-0.00132700
C	-0.32557100	1.63330000	0.02191700
O	1.02513400	-0.29828200	0.54115800
C	-0.68128700	2.30721800	-1.32256900
C	-0.24958000	2.85688700	0.96858300
C	-1.43394800	0.67397600	0.50531300
C	-1.74174200	3.36175700	-0.94640700
H	0.23665000	2.78249200	-1.68481700
H	-1.02170000	1.59656500	-2.08038900
C	-1.37796000	3.81184500	0.50127100
H	-0.33734000	2.56734400	2.01856600
H	0.73391700	3.31294700	0.81114500
O	-1.94237300	0.67109400	1.60304700
O	-1.77826500	-0.15683700	-0.50656200
H	-1.76058100	4.19598300	-1.65720300
H	-2.74100200	2.90801200	-0.96157600
H	-2.24807800	3.73247700	1.16167900
H	-1.04510300	4.85590200	0.53142500
I	-3.16958300	-1.63290400	-0.08866700
Cs	3.82727400	-0.82686200	-0.01141800

BCTC-4d



C	3.58503900	0.62791200	-0.00779000
O	4.08580700	0.89023800	-1.12393900
O	3.35869100	-0.58657000	0.38857700
C	1.82887000	1.80831500	1.41321600
O	1.04189500	2.02985100	0.35515800
O	1.44582500	1.68112000	2.55984500
C	-3.58434200	-0.62807500	-0.00775000
O	-4.08522100	-0.89006500	-1.12391000
O	-3.35794400	0.58631000	0.38895700
C	-1.82826600	-1.80857900	1.41329800
O	-1.04107800	-2.03056600	0.35549000
O	-1.44546800	-1.68085800	2.55994900
I	-1.04176700	1.56517600	0.58267600
I	1.04255200	-1.56572400	0.58326500
Cs	-4.03468400	1.86108000	-2.22235900
Cs	4.03290000	-1.85988700	-2.22427000
C	3.32191800	1.76961300	0.99619900
C	3.74130800	3.16652400	0.48616600
C	4.20920600	1.59548900	2.25587800
C	3.84969800	4.00686700	1.77288700
H	4.71645100	3.06727600	-0.00362800
H	3.04172200	3.56985800	-0.25074300
C	4.34173800	3.01502600	2.86932900
H	3.78284100	0.86346300	2.94366500
H	5.18957200	1.22352500	1.93168800
H	4.51783700	4.86717400	1.64827200
H	2.86344100	4.40408600	2.04343200
H	3.73077400	3.10180300	3.77281600
H	5.38018300	3.21869700	3.15694500
C	-3.32122200	-1.77006400	0.99591300
C	-3.74027900	-3.16688500	0.48535600
C	-4.20887500	-1.59649500	2.25538900
C	-3.84879600	-4.00765600	1.77179600
H	-4.71534600	-3.06763400	-0.00458500
H	-3.04048800	-3.56988500	-0.25153600
C	-4.34094200	-3.01619300	2.86855100
H	-3.78301500	-0.86439800	2.94341500
H	-5.18933400	-1.22493000	1.93100400
H	-4.51691400	-4.86792600	1.64682000
H	-2.86256400	-4.40497500	2.04229200
H	-3.72976300	-3.10297600	3.77189100
H	-5.37926900	-3.22019300	3.15634800

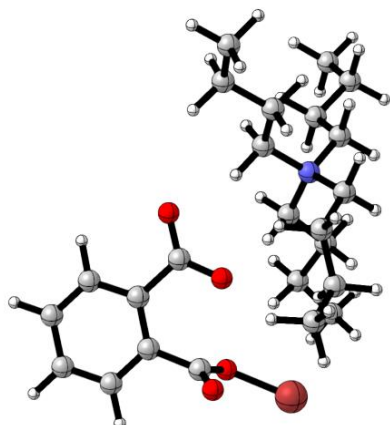
The details of the BDEs
TDRA-1



C	-6.02479000	-0.26206700	-0.30450300
C	-5.56250400	-1.51783300	-0.71138400
C	-4.20462700	-1.70444800	-0.96237000
C	-3.28982300	-0.64627600	-0.83899500
C	-3.75483000	0.62111700	-0.42339800
C	-5.12285800	0.78913400	-0.15251000
C	-2.88550100	1.83192700	-0.15845300
O	-3.35325300	2.83789700	0.39315200
O	-1.63047000	1.80063300	-0.48318800
C	-1.84874000	-0.97777500	-1.15480500
O	-1.45260500	-2.15926800	-1.09505900
O	-1.06329000	-0.01898200	-1.50444100
H	-7.08082100	-0.10409400	-0.10013500
H	-6.25509000	-2.34779900	-0.82813300
H	-3.82140100	-2.67535700	-1.25893400
H	-5.45696000	1.76434700	0.18622500
N	2.05725000	0.15857300	0.48599600
C	1.42414000	0.10172900	1.87764300
C	1.74486900	-1.09914300	-0.32165400
C	1.49610200	1.34080700	-0.32411500
C	3.55469700	0.32240600	0.70712700
H	1.92359000	-0.71785900	2.40019800
H	1.73829800	1.02873000	2.35998200
C	-0.10142900	-0.05962000	1.95350200
H	2.13931800	-0.91411500	-1.32370700
H	0.66258800	-1.13612500	-0.42887700
C	2.27765000	-2.41425000	0.23582400
H	2.15009800	1.43171800	-1.19354800
H	0.51932900	1.02564300	-0.68519800
C	1.37550800	2.67314900	0.40739500
H	3.84792200	-0.45470400	1.41741000
H	3.68298000	1.28612500	1.20607600
C	4.44865300	0.25099900	-0.53034800
H	-0.59039900	0.40722900	1.09367000
H	-0.42019200	0.53170900	2.82292000
C	-0.60514500	-1.50194900	2.14142500
H	1.89234900	-2.58921900	1.24676100
H	3.37410000	-2.41404300	0.30388800
C	1.82131800	-3.57128500	-0.67180000
H	2.30496600	2.94972200	0.92603900
H	0.57740700	2.61513500	1.15518900
C	1.00841400	3.77681400	-0.60034600
H	4.35555300	-0.72505900	-1.01970500
H	4.15955400	1.00799200	-1.26789900
C	5.91889400	0.47416700	-0.13697900
H	-0.47594600	-2.07936700	1.22075600
H	-0.00802500	-1.99547300	2.92387400

C	-2.08602700	-1.53733000	2.53635700
H	2.24123900	-3.42735200	-1.67767700
H	0.73143000	-3.52704300	-0.78574100
C	2.24801600	-4.93717500	-0.12440800
H	1.83298800	3.90518800	-1.31754100
H	0.12810600	3.45135600	-1.16554000
C	0.70331400	5.10863900	0.09264500
H	6.21598100	-0.27704500	0.60868000
H	6.02256800	1.45377100	0.35059400
C	6.85990600	0.39873000	-1.34479700
H	-2.70883900	-1.05706100	1.77530200
H	-2.25582700	-1.01776400	3.48861400
H	-2.43672600	-2.56983700	2.64410800
H	1.92247000	-5.74555900	-0.78885000
H	1.80603900	-5.12069000	0.86339100
H	3.33931300	-5.00688200	-0.02108800
H	1.55438300	5.45399000	0.69569500
H	-0.16662200	5.00802600	0.75234500
H	0.47393100	5.88916200	-0.64180500
H	6.79945600	-0.58232700	-1.83225100
H	7.90120000	0.56012000	-1.04442300
H	6.60465800	1.15975400	-2.09266200

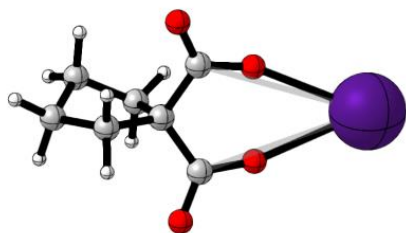
BCTC-1



C	-3.62622800	3.51652800	-2.51637200
C	-4.75566700	2.74293100	-2.22416400
C	-4.65508900	1.67738900	-1.32779300
C	-3.42542300	1.39160900	-0.72072100
C	-2.28552900	2.15672100	-1.01156200
C	-2.40289900	3.22217700	-1.91127200
C	-0.95392200	1.83944000	-0.34532400
O	0.05404700	2.51239100	-0.68070700
O	-0.98272500	0.88893100	0.49450600
C	-3.39779300	0.27188000	0.28719500
O	-3.05505200	-0.87631500	-0.39534800
H	-3.70223300	4.34772500	-3.21336300
H	-5.71141700	2.96769500	-2.69074000
H	-5.52747000	1.07411900	-1.09046000
H	-1.51177300	3.80696300	-2.11780500
O	-3.80008800	0.31212700	1.42104200
Br	-3.02248200	-2.44920000	0.64933800
N	2.60740700	-0.30339000	0.42130100
C	2.37386300	-0.69013300	1.88295700

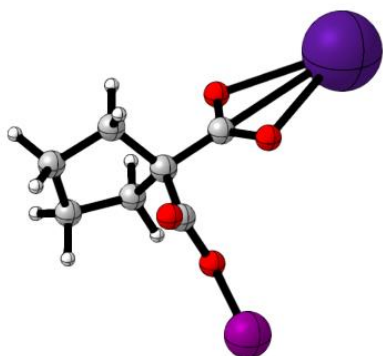
C	1.44168800	-0.75204800	-0.46035800
C	2.69462800	1.21968800	0.25525500
C	3.91511500	-0.96243800	0.00751000
H	2.32897600	-1.78228900	1.89418600
H	3.29330700	-0.40232600	2.39712100
C	1.13536200	-0.08913700	2.56848800
H	1.63320300	-0.31203200	-1.44232500
H	0.55417000	-0.25229800	-0.05862300
C	1.20935500	-2.25428900	-0.57721400
H	3.09111100	1.38077000	-0.74898600
H	1.66931600	1.60407400	0.22847400
C	3.53472500	1.96710400	1.28489700
H	3.84430200	-2.00872800	0.31539400
H	4.69597100	-0.49725100	0.61480100
C	4.28850300	-0.88557000	-1.47262500
H	0.77344000	0.79607000	2.03824400
H	1.45019900	0.24383200	3.56702100
C	-0.04288100	-1.06352700	2.71380900
H	0.92921400	-2.67791000	0.39422000
H	2.10552500	-2.79059800	-0.91763200
C	0.06432800	-2.50483400	-1.57507200
H	4.55031600	1.55433100	1.37159700
H	3.07175100	1.89910900	2.27640800
C	3.62464300	3.45084500	0.88550800
H	3.52597700	-1.37348500	-2.08962300
H	4.35065400	0.15584500	-1.80783200
C	5.64372500	-1.57045900	-1.71673300
H	-0.40983800	-1.34396300	1.72252400
H	0.30204100	-1.98550900	3.20931600
C	-1.20065800	-0.44134400	3.49779800
H	0.36352400	-2.13536400	-2.56663900
H	-0.80942000	-1.91505700	-1.27605600
C	-0.31454400	-3.98544500	-1.66737000
H	4.12805100	3.53517100	-0.08817000
H	2.60972800	3.84260800	0.74219900
C	4.37225800	4.28947600	1.92760200
H	5.59173500	-2.61515300	-1.37828600
H	6.41606100	-1.08390200	-1.10417800
C	6.05646300	-1.52938000	-3.19258300
H	-1.58716700	0.43168900	2.96411400
H	-0.88041900	-0.13574300	4.50377300
H	-2.02910800	-1.14972500	3.60289900
H	-1.13348200	-4.13684100	-2.37938200
H	-0.65012500	-4.36312700	-0.69400700
H	0.53668100	-4.59765100	-1.99458200
H	5.39799100	3.92505300	2.07281000
H	3.86428300	4.25460100	2.89970600
H	4.43078600	5.33986400	1.62022500
H	5.31690300	-2.03779000	-3.82365200
H	7.02334000	-2.02154700	-3.34631200
H	6.14534800	-0.49570900	-3.54939900

TDRA-4



C	-4.38459900	0.13703500	-0.11154400
C	-3.15366500	0.19589200	-1.04557200
C	-1.89787900	0.10789400	-0.13702600
C	-2.47278700	-0.00237700	1.32699400
C	-3.87187000	-0.60238700	1.13378700
H	-4.69477900	1.15351100	0.16576700
H	-5.24381800	-0.35537900	-0.58122600
H	-3.13013000	1.11396200	-1.63977500
H	-3.15096000	-0.66272400	-1.72488100
H	-1.81852600	-0.58507900	1.98386400
H	-2.55850700	1.00858300	1.74558600
H	-3.79153800	-1.67730000	0.92940600
H	-4.51012500	-0.46754800	2.01574900
C	-1.00086700	1.34908900	-0.20436100
C	-1.06995500	-1.16096100	-0.39255200
O	0.25751500	1.14911200	0.08154200
O	-1.55832500	-2.21079400	-0.81235400
O	-1.43498200	2.47451900	-0.45059800
O	0.19233500	-1.07712600	-0.06897700
Cs	2.84283200	-0.04288800	0.06709500

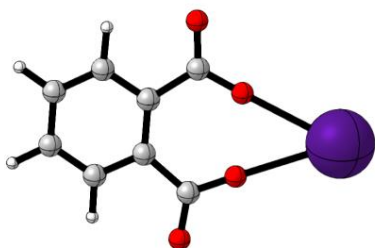
BCTC-4



O	2.00250300	1.42530600	-0.53416500
C	1.01260200	0.84491100	-0.00132700
C	-0.32557100	1.63330000	0.02191700
O	1.02513400	-0.29828200	0.54115800
C	-0.68128700	2.30721800	-1.32256900
C	-0.24958000	2.85688700	0.96858300
C	-1.43394800	0.67397600	0.50531300
C	-1.74174200	3.36175700	-0.94640700
H	0.23665000	2.78249200	-1.68481700
H	-1.02170000	1.59656500	-2.08038900
C	-1.37796000	3.81184500	0.50127100
H	-0.33734000	2.56734400	2.01856600
H	0.73391700	3.31294700	0.81114500

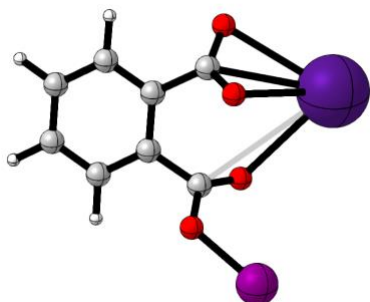
O	-1.94237300	0.67109400	1.60304700
O	-1.77826500	-0.15683700	-0.50656200
H	-1.76058100	4.19598300	-1.65720300
H	-2.74100200	2.90801200	-0.96157600
H	-2.24807800	3.73247700	1.16167900
H	-1.04510300	4.85590200	0.53142500
I	-3.16958300	-1.63290400	-0.08866700
Cs	3.82727400	-0.82686200	-0.01141800

TDRA-3



C	-4.55142700	-0.69876900	0.00006100
C	-4.55142800	0.69876700	0.00004000
C	-3.34004800	1.38587100	0.00000500
C	-2.10828700	0.70804100	-0.00000900
C	-2.10828600	-0.70804200	0.00001000
C	-3.34004700	-1.38587300	0.00004300
C	-0.89236300	-1.61200000	-0.00000400
O	-1.01796500	-2.84272100	-0.00001600
O	0.29344000	-1.08417200	0.00001000
C	-0.89236600	1.61200000	-0.00004400
O	0.29343800	1.08417400	-0.00002100
O	-1.01796800	2.84272100	-0.00008900
H	-5.48781100	-1.25111500	0.00008900
H	-5.48781200	1.25111200	0.00005200
H	-3.31880300	2.47048800	-0.00001400
H	-3.31880100	-2.47048900	0.00005400
Cs	2.90747600	0.00000000	0.00000200

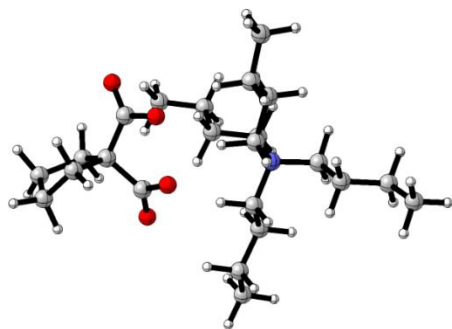
BCTC-3



C	2.14572900	0.39346300	0.76889300
O	1.24876800	-0.15789600	1.47265600
O	3.22629000	-0.12251800	0.37609600
C	-0.45618800	0.97874900	-0.38555600
O	-0.29010000	-0.02081200	-1.06317800
C	1.82038500	1.79632200	0.27782100
C	2.77057100	2.82031400	0.31165100
C	2.43622900	4.11940000	-0.08221800
C	1.14512600	4.40807600	-0.53771100

C	0.18935600	3.39175300	-0.60034100
C	0.53302800	2.09204800	-0.20690400
H	3.77230500	2.58067700	0.65621400
H	3.18280800	4.90838200	-0.03286400
H	0.88309700	5.41701700	-0.84483800
H	-0.81342400	3.59844800	-0.96300800
Cs	1.37299900	-2.53581800	-0.21324000
O	-1.59251100	1.28238400	0.26663600
I	-3.14688100	-0.09216200	0.13625000

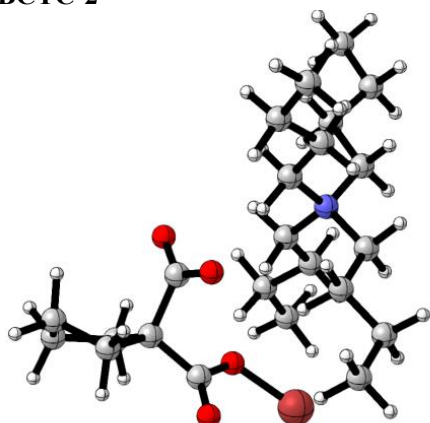
TDRA-2



C	-5.55742900	0.73932400	-0.42859600
C	-4.25443300	0.47852100	0.36934700
C	-3.26865300	-0.21683400	-0.59819000
C	-4.10619400	-0.48055600	-1.89968400
C	-5.12965200	0.66220600	-1.90425200
H	-6.29055600	-0.05148300	-0.21986900
H	-6.02479700	1.69584000	-0.16761100
H	-4.43142400	-0.15305200	1.24405100
H	-3.80851900	1.41969000	0.70630900
H	-3.47154500	-0.53459700	-2.78850000
H	-4.62610700	-1.44218600	-1.79534200
H	-4.64315700	1.59841700	-2.20841200
H	-5.96562000	0.47766200	-2.58996100
C	-2.71356800	-1.55718700	-0.09121700
C	-2.05601000	0.65044600	-0.97649500
O	-1.61019600	-1.95120300	-0.65702000
O	-1.96861500	1.86184500	-0.71195600
O	-3.27449000	-2.23508700	0.77555900
O	-1.11935200	0.00926800	-1.59642900
N	1.97288500	0.12808700	0.40664900
C	1.33879400	0.08103500	1.79380900
C	1.56632200	-1.09595000	-0.42208300
C	1.48652400	1.35416900	-0.37819000
C	3.47829000	0.18045600	0.62628600
H	1.75558500	-0.80168900	2.28427600
H	1.71937300	0.95599500	2.32712900
C	-0.18340200	0.03750600	1.83699400
H	2.05267600	-0.96723100	-1.39163200
H	0.49506400	-1.00934600	-0.59706000
C	1.89830900	-2.45575000	0.18025000
H	2.06910500	1.36223600	-1.30180000
H	0.45624000	1.14381600	-0.66266900
C	1.57522900	2.70481000	0.32407300
H	3.71457400	-0.61955600	1.33199300
H	3.67739100	1.12823700	1.13213400

C	4.36045500	0.04737600	-0.61372300
H	-0.55201400	-0.84761000	1.31160300
H	-0.61466800	0.90995400	1.33516900
C	-0.66430800	-0.00329700	3.29742700
H	1.34689800	-2.60160200	1.11682500
H	2.96887300	-2.55367900	0.40984200
C	1.48093300	-3.56489800	-0.80211100
H	2.60498200	2.94978500	0.62017000
H	0.96366400	2.70643600	1.23361200
C	1.03448800	3.79662600	-0.61778600
H	4.23652000	-0.94309800	-1.06644500
H	4.08350200	0.78584700	-1.37499200
C	5.83930400	0.24468100	-0.23982700
H	-0.24211600	-0.88836600	3.79594400
H	-0.27665800	0.87391900	3.83737200
C	-2.19373200	-0.03985600	3.39605700
H	2.03732300	-3.44484000	-1.74325100
H	0.41831400	-3.43930200	-1.03993300
C	1.72816500	-4.96492200	-0.23053800
H	1.64114400	3.82065300	-1.53485700
H	0.01436700	3.52373300	-0.91437200
C	1.04041800	5.18035300	0.04036700
H	6.11939600	-0.47944200	0.53848800
H	5.97477000	1.24237500	0.20109300
C	6.76932300	0.08518500	-1.44794400
H	-2.60185400	-0.91273500	2.87500300
H	-2.63467800	0.85356300	2.93864100
H	-2.51683600	-0.07930800	4.44300300
H	1.43151700	-5.73901300	-0.94726700
H	1.14624900	-5.12164200	0.68625100
H	2.78836600	-5.11981200	0.01172300
H	2.05354300	5.48011500	0.34081300
H	0.40691800	5.19089500	0.93631600
H	0.65517800	5.94260800	-0.64632600
H	6.67819100	-0.91591800	-1.88739300
H	7.81679200	0.23138700	-1.16164800
H	6.53002800	0.81649300	-2.23002700

BCTC-2

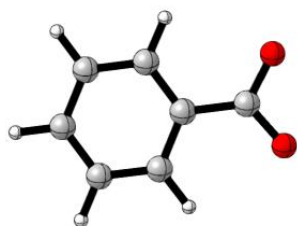


C	-3.70548000	2.70020300	-2.63676500
C	-3.62746800	2.35429400	-1.14331000
C	-2.75590900	1.07523900	-1.14419600
C	-3.18011200	0.30062100	-2.42790200

C	-3.93900400	1.33136500	-3.30991300
H	-4.49560900	3.42671800	-2.86134000
H	-2.75102500	3.12627800	-2.96923900
H	-4.62526600	2.12310200	-0.74890900
H	-3.18796400	3.13358200	-0.51530000
H	-2.27925900	-0.07389100	-2.91943100
H	-3.81767600	-0.55752000	-2.18513600
H	-3.59577800	1.31282100	-4.35020600
H	-5.01307900	1.10338800	-3.31727400
C	-2.98226900	0.26274000	0.12136600
C	-1.22449200	1.49605100	-1.13997700
O	-0.84509000	1.99034300	-0.03801700
O	-3.70207300	0.48694500	1.05819200
O	-0.54215200	1.28895600	-2.16609600
N	2.13053000	-0.16619300	0.37891900
C	1.70274100	-0.34768800	1.83690100
C	1.12302400	-0.84410700	-0.55783700
C	2.13942700	1.31513100	-0.01523200
C	3.51103900	-0.78225100	0.24891700
H	1.57425600	-1.42411600	1.97530000
H	2.55855900	-0.04205000	2.44535800
C	0.44665400	0.40079100	2.27133100
H	1.35851300	-0.49388200	-1.56290000
H	0.15887400	-0.41024100	-0.31435300
C	1.04846500	-2.36667600	-0.50335600
H	2.41286600	1.34190700	-1.07133300
H	1.09533500	1.65098900	0.03384500
C	3.05912300	2.21478100	0.80236100
H	3.43057100	-1.80528100	0.62508000
H	4.15813800	-0.23640900	0.93937200
C	4.11937100	-0.77629400	-1.15133300
H	-0.37549000	0.23120400	1.57608000
H	0.61449600	1.48189400	2.25312300
C	0.02091800	-0.02932100	3.68219300
H	0.70739600	-2.70564100	0.48225700
H	2.02510800	-2.83224800	-0.68928200
C	0.05557700	-2.86757200	-1.56829900
H	4.11719200	1.94787500	0.66795800
H	2.84183100	2.13209900	1.87478600
C	2.85156100	3.67757800	0.37097600
H	3.46037200	-1.28604000	-1.86322300
H	4.24126400	0.25210900	-1.51040300
C	5.48985500	-1.47285600	-1.14507900
H	-0.16984900	-1.11200200	3.69059700
H	0.83978800	0.15119100	4.39545200
C	-1.24099400	0.71531800	4.13542100
H	0.42296200	-2.58393400	-2.56423700
H	-0.90362700	-2.35610700	-1.43728300
C	-0.14821400	-4.38411600	-1.49724200
H	3.06245400	3.77183100	-0.70329800
H	1.79366400	3.93891100	0.49815000
C	3.73615100	4.64870300	1.15992700
H	5.37256400	-2.50641400	-0.78912400
H	6.15288300	-0.97060600	-0.42612500
C	6.14447900	-1.47808600	-2.53125400
H	-2.06943900	0.53881900	3.44032400
H	-1.06542100	1.79757900	4.17060300

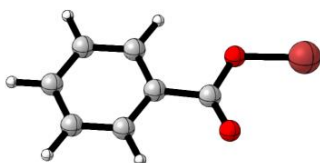
H	-1.55429400	0.38979200	5.13448500
H	-0.84575200	-4.72398700	-2.27127700
H	-0.56150600	-4.67747600	-0.52405900
H	0.79790600	-4.92381100	-1.63824200
H	4.80149700	4.41963400	1.02388400
H	3.51832400	4.59767300	2.23464500
H	3.57291100	5.68299400	0.83619700
H	5.51547100	-2.00067600	-3.26263100
H	7.11839000	-1.97977000	-2.50687100
H	6.30209800	-0.45594700	-2.89734100
O	-2.18812200	-0.87369200	0.01888200
Br	-2.26501500	-2.09241400	1.45197200

Benzoic radical



C	-2.53678800	0.00005800	0.00002600
C	-1.84124200	1.21532100	0.00004200
C	-0.44663400	1.21872400	0.00001300
C	0.24732100	-0.00002600	-0.00003700
C	-1.84132100	-1.21525600	-0.00002400
C	1.72001300	-0.00015600	-0.00007000
O	2.44054500	-1.04360400	0.00012900
H	-3.62368700	0.00013300	0.00004800
H	-2.38585400	2.15527700	0.00007900
H	0.10894200	2.15237800	0.00002400
H	-2.38596600	-2.15519000	-0.00004200
O	2.44069900	1.04365000	-0.00005100
C	-0.44671500	-1.21875300	-0.00005500
H	0.10881100	-2.15243500	-0.00009900

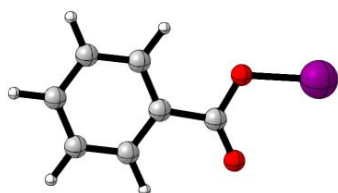
Benzoic hypobromous anhydride



C	-4.01161000	0.44531200	0.00001700
C	-3.59916500	-0.89192700	0.00006600
C	-2.24009000	-1.20359100	0.00004800
C	-1.28600000	-0.17348100	-0.00001100
C	-3.06162300	1.47230400	-0.00004700
C	0.15129600	-0.58235900	-0.00003600
O	0.95840200	0.52836400	0.00007900
H	-5.07142500	0.68659800	0.00002800
H	-4.33571000	-1.69075400	0.00011500
H	-1.90109000	-2.23445100	0.00007800
H	-3.38127600	2.51076900	-0.00008800
O	0.55562100	-1.72097700	-0.00012400

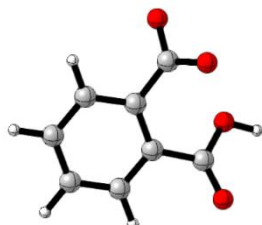
Br	2.80056700	0.19703700	0.00001300
C	-1.69954100	1.16858100	-0.00005900
H	-0.96214800	1.96342200	-0.00010700

Benzoic hypiodous anhydride



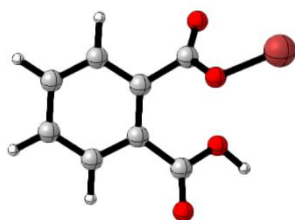
C	-4.53235800	-0.47251100	-0.00016100
C	-4.13399500	0.86899100	-0.00024100
C	-2.77802800	1.19513300	-0.00041400
C	-1.81305800	0.17559800	-0.00051800
C	-3.57123400	-1.48913100	-0.00025500
C	-0.37547900	0.59269800	-0.00072500
O	0.44342100	-0.49010700	-0.00028700
H	-5.58960200	-0.72507800	-0.00002400
H	-4.87901900	1.66003400	-0.00016900
H	-2.44975000	2.22941300	-0.00048100
H	-3.87965100	-2.53108200	-0.00019100
O	0.00711100	1.74393200	-0.00030100
C	-2.21247700	-1.17019800	-0.00042900
H	-1.46427300	-1.95485600	-0.00050400
I	2.47467600	-0.13042500	0.00042500

TDRA-H



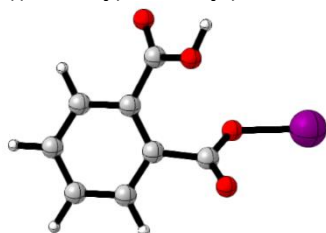
C	2.65885600	0.79114900	0.02693700
C	2.70760000	-0.60545000	0.00295700
C	1.52446400	-1.34823400	-0.01082900
C	0.28098700	-0.70805700	0.00188200
C	0.23299800	0.70299900	-0.00347300
C	1.42487700	1.44287600	0.01620100
C	-1.02367600	1.48065400	-0.14180300
O	-1.25919800	2.52236000	0.53299700
O	-1.91214200	1.23611400	-1.00315300
C	-0.92808100	-1.58635400	0.07940100
O	-0.98527600	-2.70740500	-0.38361300
H	3.57676800	1.37174700	0.04096500
H	3.66520400	-1.11837300	-0.00037200
H	1.54826100	-2.43332000	-0.01706600
H	1.37250400	2.52741900	0.00409700
O	-1.93481200	-1.01868700	0.77810300
H	-2.69946900	-1.62401900	0.75006000

2-((bromooxy)carbonyl)benzoic acid



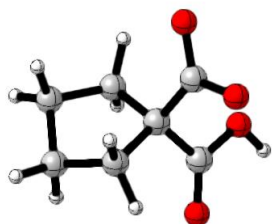
C	-3.82302500	-0.59995900	-0.45514900
C	-3.19954800	-1.83549400	-0.25798100
C	-1.83963600	-1.88869400	0.05200500
C	-1.09636800	-0.70861700	0.17321900
C	-1.72743400	0.54028300	0.00203600
C	-3.08951100	0.57946500	-0.32269100
C	-1.05046300	1.85599200	0.21374200
O	-1.37747300	2.88944900	-0.33419700
C	0.37286300	-0.87363400	0.43256800
O	1.05117500	-0.16736300	-0.52076700
H	-4.87961100	-0.55373800	-0.70328200
H	-3.76742200	-2.75704900	-0.35024800
H	-1.34057000	-2.84214300	0.19529000
H	-3.56141400	1.54772300	-0.45616500
O	0.86366800	-1.57580200	1.27886100
Br	2.91840700	-0.11501500	-0.32635100
O	-0.06410900	1.79528000	1.13974000
H	0.33741800	2.68218000	1.20109900

2-((iodooxy)carbonyl)benzoic acid



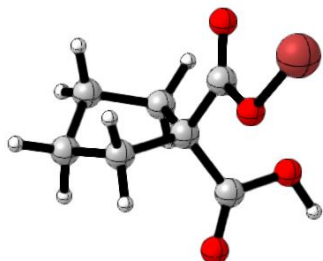
C	-4.27243100	-0.60476400	-0.49719100
C	-3.65065700	-1.83975000	-0.29173700
C	-2.29540700	-1.89165000	0.03841000
C	-1.55459300	-0.71159000	0.17343500
C	-2.18483300	0.53625800	-0.00563500
C	-3.54178400	0.57492800	-0.35169400
C	-1.51445200	1.85322900	0.21735000
O	-1.80956700	2.87815100	-0.36402100
C	-0.08619300	-0.87459800	0.44941400
O	0.61146900	-0.13233600	-0.44038200
H	-5.32510300	-0.55903500	-0.76165800
H	-4.21595900	-2.76192100	-0.39382300
H	-1.79699600	-2.84426100	0.18869700
H	-4.01254500	1.54279600	-0.49224800
O	0.38230400	-1.61629500	1.28121300
O	-0.58051800	1.80924500	1.19765700
H	-0.18635900	2.69898600	1.26517600
I	2.66621800	-0.07243500	-0.21879200

TDRA-H'



C	-2.35586400	-0.35851500	0.60788800
C	-0.99107400	-0.04062500	1.23971000
C	0.00011100	0.01620100	0.02875100
C	-0.90221200	0.16370100	-1.25118100
C	-2.32126400	0.42358400	-0.71298500
H	-2.43312200	-1.43544800	0.40958700
H	-3.19018500	-0.07680200	1.25919600
H	-0.66294000	-0.77378500	1.97918600
H	-1.02643400	0.94051900	1.72743100
H	-0.53350300	0.95224400	-1.91333400
H	-0.87597100	-0.77225600	-1.81991700
H	-2.45874500	1.49526400	-0.51778600
H	-3.09380600	0.11397300	-1.42515400
C	0.82760400	-1.26530000	-0.08437200
C	0.92845500	1.19609300	0.20665100
O	1.81216200	1.25357400	1.10905400
O	0.62873300	-2.29178100	0.52483000
O	0.87381000	2.26163400	-0.46553500
O	1.79496500	-1.13314800	-1.02215800
H	2.28281000	-1.97676900	-1.07551900

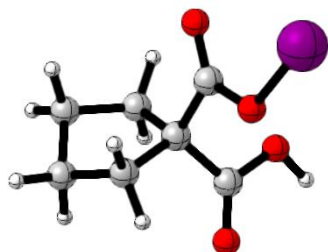
1-((bromooxy)carbonyl)cyclopentane-1-carboxylic acid



C	-2.96290800	-1.60777300	0.43508100
C	-2.25762300	-0.42378100	1.11585800
C	-1.20552700	0.07405600	0.06305000
C	-1.60829000	-0.60419000	-1.28937000
C	-3.01040500	-1.18680200	-1.04140100
H	-2.36007200	-2.51816000	0.54984300
H	-3.95101700	-1.80422100	0.86559900
H	-1.77918800	-0.67475100	2.06432900
H	-2.97953600	0.37961000	1.30429700
H	-1.56637300	0.11395200	-2.11091300
H	-0.90460600	-1.41370800	-1.51459400
H	-3.77019400	-0.40752900	-1.18621200
H	-3.24382600	-2.01159300	-1.72342900
C	0.20934600	-0.38679500	0.45078800
C	-1.27001000	1.59703900	-0.01584500
O	0.49647600	-1.20261800	1.28644000
O	-1.78027000	2.24180000	-0.90462600

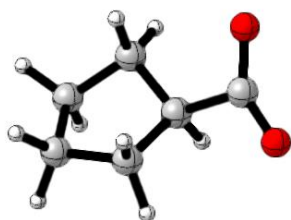
O	1.08633300	0.24240500	-0.38359900
Br	2.90116700	-0.20334600	-0.18111100
O	-0.74248100	2.16249700	1.09769000
H	-0.83397400	3.13030500	1.01375300

1-((iodooxy)carbonyl)cyclopentane-1-carboxylic acid



C	-3.38227900	-1.65490500	0.42553300
C	-2.72179900	-0.44383600	1.10307900
C	-1.67193400	0.07413000	0.05928900
C	-2.04571900	-0.61783200	-1.29430700
C	-3.43013400	-1.24511400	-1.05419800
H	-2.75050900	-2.54379300	0.55204500
H	-4.36740400	-1.88084100	0.84859100
H	-2.24862000	-0.67123000	2.06006900
H	-3.47039100	0.33914300	1.27371200
H	-2.02242100	0.10068300	-2.11624600
H	-1.31524900	-1.40439800	-1.51515700
H	-4.21421000	-0.49244200	-1.21048100
H	-3.63058700	-2.08142500	-1.73280300
C	-0.24628500	-0.35401500	0.45654100
C	-1.76651100	1.59429800	-0.02608900
O	0.03618600	-1.18419200	1.28604000
O	-2.26816300	2.22781000	-0.92818200
O	0.62815500	0.30026100	-0.33731500
O	-1.27843100	2.17450600	1.09839200
H	-1.38778800	3.13965900	1.00660800
I	2.64251300	-0.12771300	-0.11579100

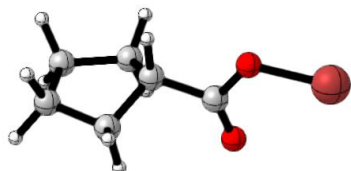
Cyclopentanecarboxylic radical



C	2.15337500	0.62405100	0.27458800
C	0.74622600	1.21726200	0.07904600
C	0.54180900	-1.19038600	-0.26916800
C	2.05310500	-0.80987100	-0.31497400
H	2.93224400	1.22604700	-0.20521300
H	2.39246700	0.57909800	1.34532100
H	0.59313100	1.51058100	-0.96560600
H	0.53789800	2.08872800	0.70652300
H	0.32600600	-2.11491700	0.27275300
H	0.14429000	-1.31846600	-1.28276300
H	2.66267800	-1.52339400	0.24928200

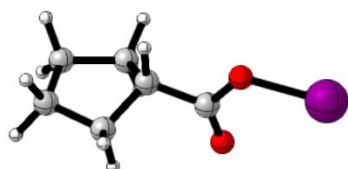
H	2.41402600	-0.82644700	-1.34894300
C	-1.69353500	0.03393000	0.02252600
O	-1.93249200	1.13180900	-0.51997600
O	-2.29350500	-0.98608500	0.32975300
C	-0.13220400	0.01415700	0.41603100
H	-0.20742000	-0.12186800	1.50213500

Cyclopentanecarboxylic hypobromous anhydride



C	-3.65591500	0.82363200	-0.17670700
C	-2.22371700	1.17875600	0.27072800
C	-2.23613800	-1.21446900	-0.05462800
C	-3.69964400	-0.73291200	-0.24517500
H	-4.40827800	1.23689300	0.50351500
H	-3.85134700	1.25174100	-1.16751500
H	-2.13128300	1.13571500	1.36270400
H	-1.89980400	2.17217000	-0.05789700
H	-1.97089600	-2.05584100	-0.70324000
H	-2.06163300	-1.52394300	0.98184100
H	-4.10026500	-1.06655300	-1.20877900
H	-4.34805500	-1.15545800	0.52979900
C	-0.00301300	-0.05394500	0.29771400
O	0.22129600	-0.22886900	1.46923700
C	-1.37849200	0.04039600	-0.34091800
H	-1.27521600	0.19248200	-1.42064000
O	0.94469700	0.09594300	-0.67643000
Br	2.74001000	0.01792700	-0.10480900

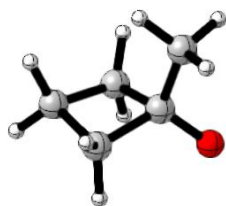
Cyclopentanecarboxylic hypoiodous anhydride



C	-4.18988800	0.80767400	-0.19529600
C	-2.74838400	1.19234000	0.20421500
C	-2.75922400	-1.21183800	0.02066400
C	-4.21463100	-0.75147800	-0.24632600
H	-4.92352800	1.21554200	0.50829000
H	-4.42937400	1.22333400	-1.18133600
H	-2.63788800	1.21977600	1.29480700
H	-2.43417300	2.16409500	-0.19164900
H	-2.47655700	-2.10242400	-0.55057900
H	-2.60964200	-1.43360800	1.08351200
H	-4.55500200	-1.09747600	-1.22891600
H	-4.90093300	-1.17674100	0.49378700
C	-0.52067000	-0.03248600	0.28950400
O	-0.30575900	-0.13612300	1.47599700
C	-1.90417700	0.02196800	-0.34452700
H	-1.80605000	0.10760400	-1.43177200
O	0.42489200	0.05483900	-0.67395000

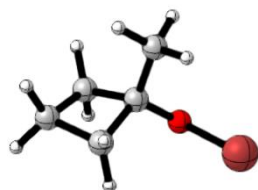
I 2.41211200 0.00703900 -0.06758400

1c-IM



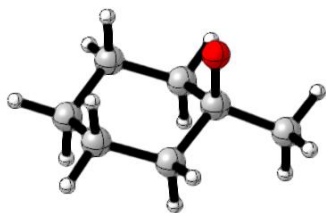
C	-1.67222900	0.27149000	-0.08842200
C	-0.69853800	0.06598600	1.10002500
C	0.49008800	-0.13479600	0.10346900
C	-0.63960700	-0.35418800	-1.05276900
H	-2.63740000	-0.24020700	-0.02968900
H	-1.84951000	1.32954100	-0.30678900
H	-0.88716600	-0.86462800	1.64309100
H	-0.59557000	0.89416900	1.80995100
H	-0.79663400	-1.42012400	-1.22878600
H	-0.39724100	0.15510600	-1.98945100
C	1.31989300	1.12773000	-0.16800500
H	1.95571200	1.34133900	0.69892400
H	1.95967600	0.97425400	-1.04303400
H	0.67362200	1.99626200	-0.34160300
O	1.22210800	-1.25287900	0.17770000

1c-Br



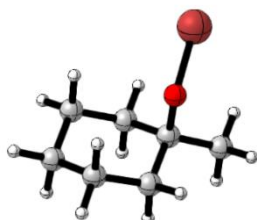
C	2.81527000	-0.71839100	-0.24969700
C	1.39622100	-0.81347700	-0.87871800
C	0.93272800	0.29796600	0.09920600
C	2.20105200	0.03084000	0.96554600
H	3.32499300	-1.66210200	-0.03624000
H	3.48707900	-0.08024600	-0.83309800
H	0.90218400	-1.76110900	-0.64369100
H	1.29333300	-0.60490000	-1.94846300
H	1.96989300	-0.64193400	1.79653700
H	2.71503200	0.91877800	1.34705900
C	0.87117600	1.69586600	-0.49914600
H	0.05974800	1.77112500	-1.23118200
H	0.70603100	2.43739400	0.29017900
H	1.81150900	1.93150900	-1.01100600
O	-0.20747500	0.00138400	0.91308800
Br	-1.82596200	-0.15075500	-0.04737000

1d-IM



C	-2.04976600	0.00151100	-0.30881100
C	-1.30114700	-1.27381400	0.10761900
C	0.15315000	-1.25784500	-0.37280800
C	0.94911700	0.03512800	0.07815800
C	0.13065900	1.29083800	-0.33677300
C	-1.31222900	1.25707500	0.17964000
H	0.70159800	-2.13853200	-0.02197500
H	-1.32175000	-1.37130200	1.19996000
H	-1.80078300	-2.16100300	-0.30458700
H	-2.13299300	0.03199700	-1.40671100
H	-3.07405100	-0.01734400	0.08498400
H	0.65771300	2.17813300	0.03622000
H	0.13708500	1.35109400	-1.43473100
H	-1.29906300	1.26932800	1.27696400
H	-1.84112400	2.16199900	-0.14691100
H	0.19653900	-1.25127700	-1.47110800
O	1.01706200	-0.07717900	1.44326100
C	2.35181700	0.02692900	-0.55435600
H	2.91998000	0.89841500	-0.20944300
H	2.89450600	-0.87635000	-0.25587900
H	2.29624100	0.06333300	-1.64887900

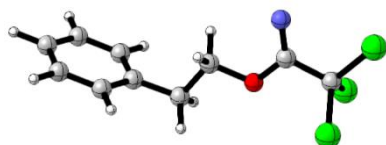
1d-Br



C	-2.75002500	-1.06811500	0.02315000
C	-2.41422700	-0.13537900	-1.15096100
C	-1.70792600	1.14206900	-0.67128000
C	-0.46064200	0.85823500	0.20190500
C	-0.82457000	-0.09745700	1.35044100
C	-1.49684500	-1.38454900	0.85365900
H	-1.41113500	1.76849900	-1.52078500
H	-1.76260400	-0.66064100	-1.85981900
H	-3.32734800	0.13840600	-1.69540700
H	-3.49951300	-0.58470000	0.66968600
H	-3.20547300	-1.99489200	-0.34896600
H	0.07596300	-0.32635600	1.93315000
H	-1.50535700	0.44129600	2.02498300
H	-0.78185800	-1.94817400	0.23999900
H	-1.75389200	-2.02022400	1.71060700
H	-2.39389500	1.73795600	-0.05218400
C	0.16778700	2.15535800	0.70817800
H	1.06736100	1.94979800	1.29862100
H	0.44506300	2.79821300	-0.13419100

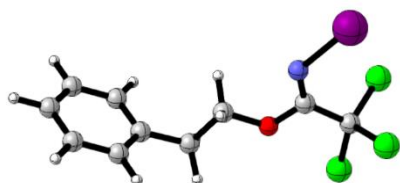
H	-0.53926200	2.69726200	1.34651900
O	0.40790800	0.21708400	-0.77672000
Br	2.06421100	-0.41583100	-0.15111400

3a-IM



N	1.32900600	-0.00046200	1.94504500
C	1.47251600	0.00003100	0.68620300
O	0.48227400	0.00021500	-0.21960300
C	-0.87332200	0.00004300	0.30089400
C	-1.81151500	0.00028900	-0.90186800
C	2.85923700	0.00000200	0.01903900
Cl	3.00989900	-1.47423200	-1.00650500
Cl	4.14349900	-0.00067600	1.26707400
Cl	3.01045700	1.47489300	-1.00547800
C	-3.25729800	0.00013400	-0.45032600
C	-3.93321000	-1.20612300	-0.21522100
C	-5.25348800	-1.20883800	0.24346400
C	-5.91742500	-0.00017300	0.47510600
C	-5.25359900	1.20864500	0.24394700
C	-3.93332100	1.20623500	-0.21473900
H	-1.01329800	-0.89004000	0.92500400
H	-1.01335900	0.88982800	0.92541600
H	-1.59616000	0.88325300	-1.51487700
H	-1.59609800	-0.88237700	-1.51528600
H	-3.42348200	-2.15014500	-0.39861100
H	-5.76347800	-2.15321000	0.41596700
H	-6.94497000	-0.00029100	0.82926900
H	-5.76367600	2.15290100	0.41682600
H	-3.42367900	2.15037600	-0.39775100

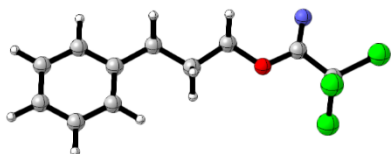
3a-I



C	0.67246900	0.44247300	-0.00018000
O	-0.51636100	1.06367000	-0.00037100
C	-1.71309800	0.24565400	-0.00025600
C	-2.89794700	1.20797500	0.00002800
C	1.82605900	1.49372100	-0.00004000
Cl	2.82399700	1.26024600	-1.48271900
Cl	2.82352700	1.26022300	1.48305300
Cl	1.22050300	3.18739700	-0.00009700
C	-4.20420300	0.44179700	0.00003500
C	-4.80991600	0.05952700	-1.20591100
C	-5.99272400	-0.68511300	-1.20862600
C	-6.58764400	-1.06011400	0.00002300
C	-5.99292200	-0.68481900	1.20867400

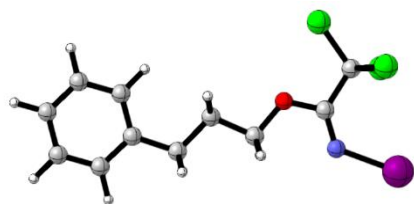
C	-4.81011000	0.05982200	1.20597100
H	-1.70373500	-0.39722800	-0.88643200
H	-1.70344900	-0.39742800	0.88576700
H	-2.82839600	1.85459700	0.88263900
H	-2.82857900	1.85488900	-0.88238600
H	-4.35408800	0.35232000	-2.14991900
H	-6.45041800	-0.96870500	-2.15302000
H	-7.50889700	-1.63687100	0.00001700
H	-6.45076800	-0.96818100	2.15306300
H	-4.35443400	0.35283800	2.14998200
N	0.69523400	-0.83335100	-0.00021300
I	2.41039200	-2.05436600	0.00004500

3b-IM



C	-1.39306600	0.28819100	-0.00033100
C	-2.66594500	1.14339300	-0.00052600
C	-0.15047300	1.16154900	-0.00043800
O	0.99583600	0.27058500	-0.00033100
C	2.20560100	0.85114200	-0.00038700
C	3.34030900	-0.18835700	0.00005400
N	2.43171100	2.09787900	-0.00033200
Cl	3.18840200	-1.21286700	1.47460500
Cl	3.18926200	-1.21320900	-1.47434600
Cl	4.93015700	0.63588100	0.00042100
C	-3.98197800	0.38050200	-0.00016000
C	-5.18188200	1.11235300	0.00034900
C	-6.42048000	0.47049900	0.00064200
C	-6.48562300	-0.92794700	0.00042500
C	-5.30211100	-1.66737100	-0.00007700
C	-4.06086800	-1.01809900	-0.00035800
H	-1.36633000	-0.36137700	0.88299900
H	-1.36624200	-0.36167100	-0.88344200
H	-2.65052900	1.80807200	-0.87684400
H	-2.65040800	1.80868400	0.87532100
H	-0.09556800	1.80036500	0.88954000
H	-0.09556900	1.80014800	-0.89057100
H	-5.14048100	2.20042300	0.00052400
H	-7.33425500	1.05966500	0.00104400
H	-7.44843100	-1.43227000	0.00065300
H	-5.33783500	-2.75403400	-0.00024200
H	-3.15688400	-1.61964700	-0.00073600

3b-I

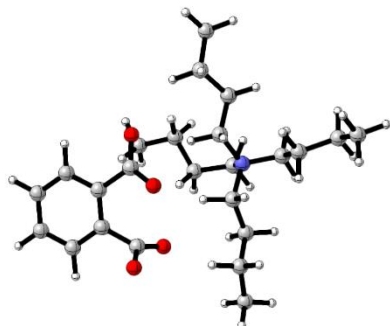


C	-2.54664400	0.01363000	-0.00123300
C	-3.61605200	-1.08509500	-0.00285600

C	-1.15210700	-0.59014400	-0.00120000
O	-0.21809100	0.51809400	-0.00079400
C	1.09327900	0.23667100	-0.00037000
C	1.92528100	1.55688800	0.00034400
N	1.45578200	-0.98692300	-0.00059200
Cl	0.89065300	3.02793700	0.00025400
Cl	2.94862300	1.59646300	1.48356100
Cl	2.94998600	1.59726300	-1.48190800
C	-5.06134000	-0.61122900	-0.00103900
C	-6.08464700	-1.57479900	0.00154000
C	-7.42918700	-1.20262300	0.00290900
C	-7.78172300	0.15225000	0.00177900
C	-6.77616100	1.11994200	-0.00074300
C	-5.42763100	0.74096900	-0.00213500
H	-2.65516800	0.65627800	-0.88351500
H	-2.65611500	0.65444500	0.88227200
H	-3.46295700	-1.73479800	0.87156300
H	-3.46392200	-1.73128100	-0.88005100
H	-0.96257000	-1.20583100	-0.88748500
H	-0.96280700	-1.20628800	0.88480900
H	-5.81939200	-2.63087400	0.00247200
H	-8.20171200	-1.96771000	0.00491300
H	-8.82790000	0.44704700	0.00286800
H	-7.03538900	2.17589600	-0.00161800
H	-4.66709500	1.51590600	-0.00411000
I	3.43383800	-1.70785100	0.00007500

SOMO-HOMO inversion

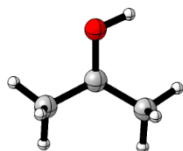
TDRA-1-SHI



C	-5.91318900	-0.06665800	-0.25432600
C	-5.51043900	-1.38191900	-0.49274000
C	-4.16851000	-1.67517700	-0.73498600
C	-3.21410500	-0.66177400	-0.76351800
C	-3.62251900	0.65200900	-0.49498100
C	-4.96851300	0.95516800	-0.25682600
C	-2.62591200	1.77315900	-0.37724400
O	-2.78171100	2.57630800	-1.40088300
O	-1.87988900	2.00759900	0.55287300
C	-1.74853600	-0.96912300	-1.06914700
O	-1.35591300	-2.13526200	-0.85258500
O	-1.07972000	0.01292900	-1.47961600
H	-6.95779100	0.16165000	-0.06658700
H	-6.24691500	-2.18048200	-0.49183000
H	-3.83059600	-2.69232600	-0.91074300
H	-5.26415300	1.98218500	-0.06130200
N	1.95960400	0.14100500	0.52180600

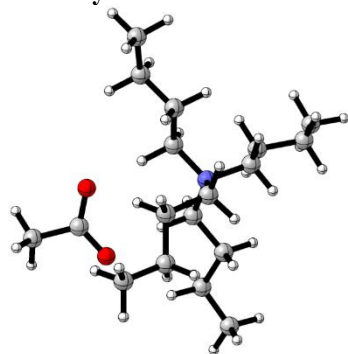
C	1.39299200	-0.09213400	1.90810800
C	1.68487600	-1.04526100	-0.38364700
C	1.29857500	1.34292500	-0.13669600
C	3.43831700	0.36595900	0.70386300
H	1.98726800	-0.90139100	2.34251600
H	1.62925900	0.81721900	2.46414700
C	-0.09931000	-0.42344100	1.98246800
H	1.93513300	-0.71872800	-1.39689100
H	0.60311700	-1.19988000	-0.38729000
C	2.41417700	-2.33073900	-0.02882300
H	1.88025900	1.53366900	-1.04254200
H	0.30980700	1.01141200	-0.46672200
C	1.18405200	2.59462000	0.71641500
H	3.81821800	-0.51885600	1.22247400
H	3.54337000	1.21345400	1.38706200
C	4.24659200	0.61185600	-0.56286700
H	-0.63664200	-0.02936800	1.11231500
H	-0.50812900	0.12886600	2.83829500
C	-0.39874300	-1.91445100	2.16919000
H	2.24581600	-2.59955500	1.02245100
H	3.50050600	-2.23712900	-0.17028900
C	1.88010600	-3.46110500	-0.91605800
H	2.13230600	2.86230700	1.20459700
H	0.42818300	2.44249700	1.49533600
C	0.73034100	3.75647900	-0.17340200
H	4.03753500	-0.15765200	-1.31523000
H	3.98627600	1.57920600	-1.00716200
C	5.74309900	0.59933600	-0.23796800
H	-0.13304000	-2.47135300	1.26371400
H	0.21410700	-2.30354400	2.99614900
C	-1.87634300	-2.15162000	2.46544200
H	2.07950200	-3.21542000	-1.96723900
H	0.78877100	-3.50432800	-0.81817900
C	2.51243700	-4.80538800	-0.56685500
H	1.53868600	4.02022800	-0.86881700
H	-0.11993600	3.42230300	-0.77887900
C	0.32059000	4.97399500	0.64905700
H	6.01527200	-0.38067900	0.17515800
H	5.95387000	1.33858500	0.54590800
C	6.59760600	0.89526300	-1.46815600
H	-2.49242700	-1.78836200	1.63761600
H	-2.18436500	-1.63169100	3.38036100
H	-2.08533200	-3.21824500	2.59060100
H	2.13191900	-5.59999800	-1.21498600
H	2.28842200	-5.08452800	0.46899800
H	3.60290600	-4.77500200	-0.67734100
H	1.14026900	5.31374000	1.29336700
H	-0.53490500	4.72624600	1.28589900
H	0.03139600	5.80919000	0.00444200
H	6.41821700	0.15574100	-2.25582100
H	7.66338000	0.87466900	-1.22415500
H	6.36525600	1.88382400	-1.87816600

Electrophilicity and Nucleophilicity Index
2-hydroxy-2-propyl radical



C	-0.00786600	0.03214400	-0.24495500
O	0.04429600	1.37301400	0.06427800
H	0.94314900	1.70584300	-0.07171200
C	1.22418700	-0.76648600	0.03571200
H	1.13178700	-1.77555300	-0.37562900
H	2.11634000	-0.30789300	-0.40965800
H	1.40932500	-0.86272900	1.12024000
C	-1.35444400	-0.54328200	0.02790400
H	-2.13762200	0.09457800	-0.39248900
H	-1.44342600	-1.54227600	-0.40837000
H	-1.54517700	-0.63034500	1.11143100

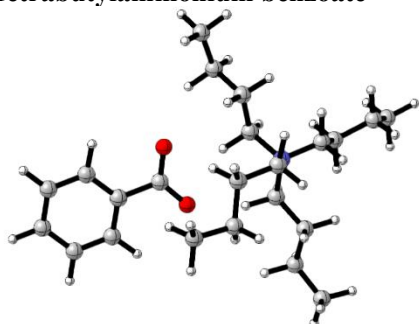
Tetrabutylammonium acetate



C	-2.93897900	0.51638800	-1.50720100
O	-2.79940900	-0.63994300	-1.02708400
O	-2.16547800	1.49413800	-1.30370900
N	0.80447300	0.05375800	0.49016300
C	0.09764800	0.17785500	1.82619400
C	0.14556900	-1.00875400	-0.36784100
C	0.69058800	1.34399500	-0.30391500
C	2.23882900	-0.28481100	0.79840900
H	0.27321800	-0.76932700	2.34459400
H	0.65351400	0.94637200	2.36783300
C	-1.39973400	0.49218900	1.76475100
H	0.58950100	-0.90806000	-1.36305200
H	-0.91355900	-0.72631400	-0.46886800
C	0.27251300	-2.43967900	0.12944800
H	1.36132900	1.22236500	-1.15861000
H	-0.33781500	1.37876600	-0.69236700
C	1.00741200	2.62432000	0.45065000
H	2.21155900	-1.18893700	1.41391100
H	2.62353400	0.52494800	1.42560800
C	3.15631200	-0.50111300	-0.39715400
H	-1.67979200	0.93634900	0.79961000
H	-1.60231100	1.25540500	2.52792300
C	-2.29374000	-0.72163600	2.03518300
H	-0.05650800	-2.52381200	1.17326500
H	1.31050300	-2.80099400	0.08656100
C	-0.61940000	-3.33748700	-0.73612800
H	2.00104600	2.60143900	0.92167100

H	0.26766400	2.78742400	1.24401300
C	0.93217700	3.80325800	-0.52511300
H	2.72225800	-1.22684000	-1.09476100
H	3.30148900	0.43405300	-0.94990900
C	4.51890100	-1.01650600	0.07506000
H	-2.16525400	-1.45967500	1.23564200
H	-1.99594300	-1.19206500	2.98462000
C	-3.76489100	-0.32257400	2.08356400
H	-0.27438000	-3.28885100	-1.77730300
H	-1.63783400	-2.93042700	-0.73503600
C	-0.61176900	-4.78524600	-0.25358000
H	1.68501900	3.67187800	-1.31351100
H	-0.04757200	3.78589700	-1.01729100
C	1.14714200	5.14221200	0.17571000
H	4.38194500	-1.96794100	0.60520700
H	4.94526500	-0.31235900	0.80147200
C	5.49077900	-1.20953200	-1.08662800
H	-4.06540200	0.08494300	1.11388200
H	-3.94563600	0.43258800	2.85813800
H	-4.40116900	-1.18685700	2.29657200
H	-1.24231600	-5.41551700	-0.88720100
H	-0.99286100	-4.85633400	0.77142900
H	0.40133300	-5.20444000	-0.26430900
H	2.12596800	5.17934800	0.66773300
H	0.38039400	5.30915100	0.93983700
H	1.09680100	5.97270900	-0.53425500
H	5.09463800	-1.92770600	-1.81243600
H	6.45693300	-1.58364400	-0.73673400
H	5.66611100	-0.26476300	-1.61208400
C	-4.17512900	0.77311700	-2.37121300
H	-4.99334100	1.09689100	-1.71699400
H	-3.98564400	1.57051700	-3.09325100
H	-4.49026500	-0.14202200	-2.87751000

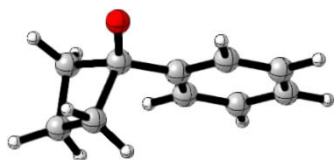
Tetrabutylammonium benzoate



C	-6.45812700	-0.36949800	-1.13610000
C	-5.53569300	-1.39322400	-1.35699400
C	-4.17984700	-1.17302700	-1.11960600
C	-3.73695000	0.06905200	-0.65992600
C	-4.66343300	1.09014100	-0.43887500
C	-6.01965500	0.87330200	-0.67659900
C	-2.25814800	0.30599900	-0.38900700
O	-1.47538500	-0.66101400	-0.60420900
O	-1.92558700	1.43650900	0.04990600
H	-7.51539900	-0.53979900	-1.32116100
H	-5.87524900	-2.36176800	-1.71455600
H	-3.44149700	-1.95193300	-1.28450900

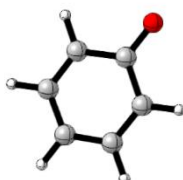
H	-6.73655200	1.67156900	-0.50362800
N	1.89656800	0.17680400	0.45852900
C	1.47733700	0.01525400	1.90891800
C	1.56467000	-1.05224300	-0.35896600
C	1.13920500	1.32607700	-0.19791500
C	3.38041100	0.44941700	0.47307400
H	2.07920800	-0.80690200	2.30764000
H	1.82012900	0.93262300	2.39378800
C	-0.00974800	-0.21084100	2.17587100
H	1.85073300	-0.80732900	-1.38700200
H	0.47117900	-1.12386100	-0.35095400
C	2.23447900	-2.34117600	0.08893200
H	1.65680600	1.51605100	-1.14186300
H	0.13580800	0.95048800	-0.41988000
C	1.01088600	2.60120700	0.61849000
H	3.82883600	-0.29633200	1.13647600
H	3.50479100	1.42656600	0.94870900
C	4.09257900	0.42740500	-0.87336900
H	-0.62737500	0.36068400	1.47337600
H	-0.19740300	0.22559800	3.16701100
C	-0.47666600	-1.66883200	2.20982600
H	1.95187600	-2.58908600	1.11872400
H	3.33048900	-2.26373700	0.06277500
C	1.78850300	-3.48536200	-0.82658800
H	1.97613500	2.95194700	1.01240700
H	0.33719600	2.42806300	1.46546000
C	0.39062100	3.68961900	-0.26272000
H	4.04853700	-0.57414500	-1.31692400
H	3.62081200	1.11549800	-1.58365800
C	5.56020400	0.82727900	-0.69379900
H	-0.37790200	-2.12886900	1.22191100
H	0.14824300	-2.24145600	2.91244300
C	-1.94356600	-1.75371000	2.62488000
H	2.07878000	-3.25778700	-1.86054300
H	0.69292000	-3.54045800	-0.81796400
C	2.38428800	-4.82536400	-0.40296400
H	1.06853100	3.91685100	-1.09718200
H	-0.53951100	3.29098700	-0.68248800
C	0.09755700	4.95995000	0.53074100
H	6.03540300	0.15515600	0.03270200
H	5.61309100	1.83688600	-0.26696700
C	6.32842500	0.78443500	-2.01272800
H	-2.57037400	-1.22819200	1.89739600
H	-2.10402900	-1.29938900	3.60960800
H	-2.28194700	-2.79316900	2.67171700
H	2.05955900	-5.63077000	-1.06773900
H	2.07425000	-5.08571700	0.61491600
H	3.47960400	-4.79459700	-0.42248400
H	1.00722000	5.36477400	0.99066100
H	-0.62368700	4.75322000	1.32827200
H	-0.32850400	5.73666400	-0.11103700
H	6.31445300	-0.22313900	-2.44182200
H	7.37314500	1.07500500	-1.87178900
H	5.88552900	1.46683800	-2.74591700
H	-4.29603200	2.04621000	-0.07866300

1a-IM



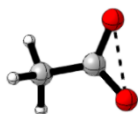
C	3.04764400	-0.32652500	0.13005300
C	2.17259700	-1.37435500	-0.14340100
C	0.80683700	-1.12911400	-0.29267000
C	0.30072500	0.16704300	-0.16813300
C	1.18586400	1.21488200	0.10583100
C	2.54836200	0.97051800	0.25292100
C	-1.18617100	0.47584300	-0.27968500
H	4.11069200	-0.51715300	0.24271000
H	2.54970300	-2.38766600	-0.24649300
H	0.14510800	-1.96177700	-0.51258200
H	3.22332900	1.79591700	0.46013100
C	-2.10248800	-0.64468700	-0.84677500
C	-2.40704800	-1.13693100	0.58198000
C	-1.93167900	0.21847300	1.13343800
H	-3.44034800	-1.41081200	0.80429000
H	-1.74812600	-1.95143300	0.89380200
H	-1.25647500	0.24711700	1.99002200
H	-2.74242000	0.93987200	1.25117300
H	-1.65216800	-1.34701200	-1.55283400
H	-2.97179900	-0.16970300	-1.30770700
O	-1.45243000	1.74100500	-0.63176200
H	0.79409500	2.22371700	0.19023500

Phenylloxy radical



C	1.77980000	0.00000200	0.00000100
C	1.08455100	1.22559500	0.00007400
C	-0.29037400	1.23982400	-0.00004500
C	-1.04507600	0.00000100	-0.00001400
C	-0.29037000	-1.23982900	0.00003300
C	1.08455200	-1.22559400	-0.00003600
H	2.86529800	0.00000600	-0.00004500
H	1.64270900	2.15679300	-0.00003500
H	-0.86066100	2.16344500	-0.00008100
H	-0.86065400	-2.16345100	0.00000300
H	1.64271900	-2.15678700	-0.00001500
O	-2.29598900	0.00000000	0.00001200

Acetyl radical



C	0.09902400	0.00148200	-0.00905500
O	0.81354500	-1.03212300	0.00184000

O	0.81532000	1.03060000	0.00184900
C	-1.39278600	0.00047900	-0.00263600
H	-1.73610900	-0.00632500	1.03629400
H	-1.76649600	0.90192000	-0.49229100
H	-1.76573900	-0.89517600	-0.50336300

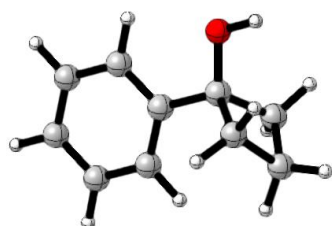
Hydroxyl



O	0.00000000	0.00000000	0.10883100
H	0.00000000	0.00000000	-0.87064800

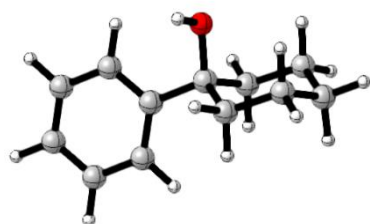
Polarity matching

1a



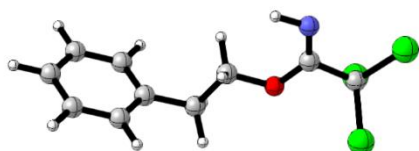
C	3.08508000	-0.38646800	0.00074300
C	2.15103900	-1.42465900	-0.00144300
C	0.78726300	-1.14135200	-0.00231300
C	0.32662200	0.18303900	-0.00099100
C	1.26928300	1.21575400	0.00125100
C	2.63751100	0.93264400	0.00207700
C	-1.15986000	0.47695600	-0.00123900
H	4.14887700	-0.60658300	0.00133800
H	2.48438100	-2.45877300	-0.00255500
H	0.07997900	-1.96715600	-0.00404300
H	3.35268900	1.75089300	0.00372200
C	-1.97128900	-0.29196900	-1.08649700
C	-2.53196800	-1.23527900	0.00373800
C	-1.96997900	-0.28678200	1.08879400
H	-3.61589600	-1.37195700	0.00473600
H	-2.05874400	-2.22020500	0.00582900
H	-1.39037000	-0.73415300	1.90142800
H	-2.74163200	0.36251100	1.51612400
H	-1.39280400	-0.74319000	-1.89781600
H	-2.74348600	0.35530800	-1.51587900
O	-1.31609200	1.88206300	-0.00449400
H	-2.26664400	2.07986700	-0.00387600
H	0.93016100	2.24561900	0.00222300

1b



C	-3.33459000	0.64631100	-0.27705300
C	-2.67423500	-0.32065300	-1.27165500
C	-1.14654000	-0.16101900	-1.27707500
C	-0.52970800	-0.31429100	0.13080000
C	-1.22659700	0.64467700	1.12677400
C	-2.75241500	0.46507300	1.13329300
H	-0.67805100	-0.89906600	-1.93901900
H	-2.92422600	-1.35299700	-0.99744200
H	-3.06219800	-0.15203800	-2.28486500
H	-3.16479600	1.68316900	-0.60844400
H	-4.42170500	0.49413700	-0.26168700
H	-0.80568200	0.48219000	2.12987700
H	-0.99103500	1.68197400	0.85944700
H	-3.00067600	-0.53912600	1.50028600
H	-3.20209900	1.18352600	1.83111000
H	-0.87559700	0.83240400	-1.65891100
O	-0.81604400	-1.67199900	0.51514600
H	-0.54425000	-1.79672600	1.43918700
C	0.98413400	-0.07625600	0.06548400
C	1.51032600	1.21714200	-0.09290300
C	1.88158400	-1.15279000	0.11218500
C	2.88783700	1.42927400	-0.18217400
H	0.84393600	2.07305800	-0.15536100
C	3.26231500	-0.94378000	0.02534900
H	1.49349100	-2.16245000	0.19947300
C	3.77280700	0.34813400	-0.11833700
H	3.26927100	2.44043300	-0.30239400
H	3.93715400	-1.79557500	0.06502700
H	4.84529300	0.51214700	-0.18556900

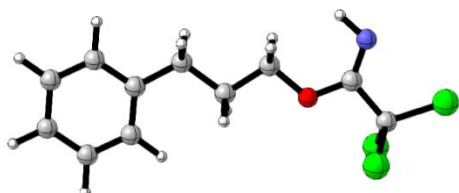
3a



C	-1.49182400	-0.08217000	0.75262600
O	-0.49341100	0.04064000	-0.13072200
C	0.87331800	-0.01258800	0.36336000
C	1.79675700	0.11474900	-0.84515700
C	-2.84105900	-0.00145300	0.00186400
Cl	-2.94391400	1.58622000	-0.85690000
Cl	-4.23406300	-0.14822800	1.10881900
Cl	-2.91870900	-1.33858700	-1.21307100
C	3.25235900	0.05420700	-0.42600700
C	3.96065400	1.22657200	-0.11716100
C	5.29710200	1.16917900	0.29285900
C	5.94609800	-0.06577200	0.40152300
C	5.25028100	-1.24094400	0.09574000
C	3.91440900	-1.17926300	-0.31446900
H	1.02217800	0.81086100	1.07036100
H	1.02320800	-0.96698800	0.87970700
H	1.57322600	-0.69736000	-1.54528300
H	1.58924700	1.06376000	-1.35086600
H	3.46368500	2.19010600	-0.20500400
H	5.83084000	2.08764700	0.52310000

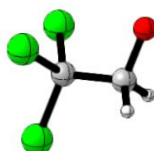
H	6.98495000	-0.11187900	0.71714600
H	5.74738500	-2.20449800	0.17240300
H	3.38124900	-2.09601400	-0.55644900
N	-1.46563000	-0.24357000	2.00991000
H	-0.51418400	-0.28075400	2.37981900

3b



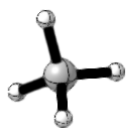
C	-1.37630100	0.32842700	-0.00019100
C	-2.66172900	1.16330400	-0.00025500
C	-0.14240000	1.21759300	-0.00022200
O	1.00637600	0.35341300	-0.00044900
C	2.23372100	0.91075700	-0.00007500
C	3.29580200	-0.21144700	0.00012800
Cl	3.05472200	-1.22991500	1.47682200
Cl	3.05551500	-1.22951400	-1.47714500
Cl	4.95240500	0.44050300	0.00062800
C	-3.96553900	0.37957000	-0.00008000
C	-5.17710000	1.09185700	0.00019800
C	-6.40509100	0.42995100	0.00034300
C	-6.44734700	-0.96937600	0.00020800
C	-5.25196200	-1.68946100	-0.00007100
C	-4.02142000	-1.02018100	-0.00021100
H	-1.33702200	-0.32097300	0.88241600
H	-1.33696200	-0.32104600	-0.88274100
H	-2.65755600	1.82836900	-0.87673600
H	-2.65747900	1.82862900	0.87602700
H	-0.11319300	1.85675000	0.89350900
H	-0.11338200	1.85693200	-0.89383300
H	-5.15354500	2.18051200	0.00030600
H	-7.32835900	1.00410700	0.00056300
H	-7.40179200	-1.48931800	0.00032300
H	-5.26992300	-2.77652600	-0.00017700
H	-3.10789000	-1.60708500	-0.00042900
N	2.58348600	2.12791500	0.00009600
H	1.79298100	2.77272400	-0.00010400

2,2,2-trichloro-ethyloxyl



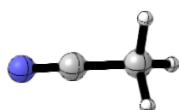
O	-2.11597700	0.00309100	0.99788800
C	-0.75956600	-0.00003800	1.35249100
C	0.09540600	-0.00024700	0.09215700
Cl	-0.26543300	1.46693000	-0.87697300
Cl	-0.27335500	-1.46375900	-0.87965600
Cl	1.83173500	-0.00435500	0.54732100
H	-0.53561100	-0.91050100	1.95224900
H	-0.53172000	0.90759300	1.95499600

Methane



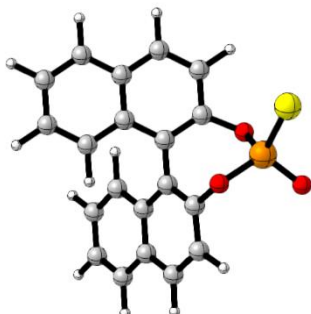
C	-0.00005400	0.00002100	0.00002700
H	0.04864100	0.92473700	-0.61746600
H	0.10761600	-0.89179700	-0.65722100
H	0.82388800	0.01030900	0.74821800
H	-0.97981900	-0.04337300	0.52630800

Acetonitrile



C	1.18650000	0.00004600	-0.00004300
H	1.55814000	-0.14897700	1.03840400
C	-0.28350000	0.00001800	0.00000900
N	-1.44150000	-0.00000500	0.00005000
H	1.55699300	-0.82555900	-0.64811200
H	1.55736700	0.97418800	-0.39043400

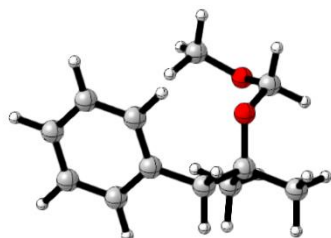
Thiyl radical (4-mercaptodinaphtho[2,1-d':1',2'-f][1,3,2]dioxaphosphepine 4-oxide)



C	2.78479200	3.38082800	-0.89282300
C	3.00413600	2.09473300	-1.18508100
C	2.10802400	1.16698600	-0.83323500
C	0.99248000	1.52531000	-0.18908800
C	0.77313500	2.81140600	0.10317000
C	1.66933400	3.73917700	-0.24872000
C	0.10189100	0.59620800	0.17286900
C	-1.01358900	0.95442400	0.81708100
C	-1.23837000	2.24190000	1.09918400
C	-0.33678200	3.16830300	0.75736100
C	0.33216200	-0.69243200	-0.09908100
C	1.52470100	-1.23097300	0.17577800
C	1.75492500	-2.51960000	-0.09625900
C	0.79265800	-3.26969800	-0.64306600
C	-0.41464000	-2.74079800	-0.87971700
C	-0.62630900	-1.43969700	-0.65641700
C	2.48310200	-0.48382800	0.73313600
C	3.67557700	-1.02226100	1.00792900
C	3.90205200	-2.31373300	0.74650900
C	2.94358100	-3.06099900	0.18917200

O	-1.96688700	0.08639700	1.23375900
O	-1.83725400	-0.96712600	-1.03906300
P	-2.90503100	-0.60394300	0.11499500
O	-3.56209100	-1.82115200	0.64141400
S	-4.49081600	0.62733200	-0.54676500
H	3.52206600	4.14413400	-1.18235300
H	3.92187400	1.79991900	-1.71506200
H	2.28848700	0.10886600	-1.07368600
H	1.48887100	4.79729700	-0.00826900
H	-2.16491000	2.53882700	1.61234300
H	-0.50830700	4.22404500	1.01452500
H	0.99256600	-4.32079000	-0.89847600
H	-1.23026700	-3.37522700	-1.25683600
H	2.29056100	0.57395000	0.96556800
H	4.47031300	-0.40284900	1.44917600
H	4.87684400	-2.76156600	0.98990300
H	3.13312200	-4.12125400	-0.03461000

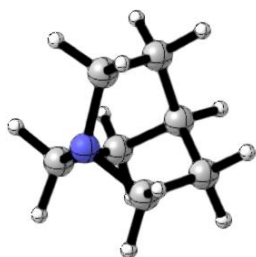
(2-(methoxymethoxy)-2-methylpropyl)benzene



C	2.68308300	0.92427000	-0.99469600
C	3.50838100	0.65691700	0.10311400
C	3.18281400	-0.39100400	0.96905100
C	2.03821500	-1.16035100	0.73761700
C	1.19787000	-0.89747000	-0.35396500
C	1.53971400	0.15354700	-1.21913300
C	-0.05804600	-1.70830200	-0.58426500
C	-1.35896000	-1.07411500	-0.02745400
O	-1.49223400	0.15743100	-0.78354600
C	-2.54629700	-1.99449900	-0.34964900
C	-1.25928900	-0.82851900	1.48435000
C	-2.42945100	1.12193700	-0.37345200
O	-1.99730300	1.93469900	0.68996200
C	-0.82511200	2.69162500	0.39915500
H	-2.61123800	1.73107900	-1.27124600
H	-0.20655800	-1.86060800	-1.66024500
H	2.93040600	1.73413100	-1.67709300
H	4.39901900	1.25531800	0.27788800
H	3.81967100	-0.61244000	1.82209700
H	1.79250800	-1.97494300	1.41602500
H	0.89156400	0.37245300	-2.06278600
H	0.05060900	-2.70088600	-0.12974200
H	-3.49104100	-1.56289800	-0.00041000
H	-2.42652900	-2.96574700	0.14458500
H	-2.62039600	-2.15770700	-1.43040100
H	-1.05675800	-1.77874600	1.99356000
H	-0.45406500	-0.12913800	1.71844500
H	-2.18988200	-0.41790700	1.88578000
H	-3.36752400	0.67247300	-0.02856300
H	-0.64928400	3.33519500	1.26448900

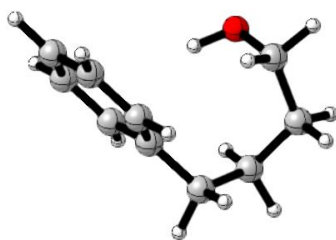
H	0.04169100	2.04091000	0.23748500
H	-0.97342300	3.31820400	-0.49522600

Quinuclidinium radical (1-Azabicyclo[2.2.1]heptane)



C	1.42334990	-0.26483431	-0.78811160
C	-0.38680489	1.39112280	0.74017217
C	1.39480583	-0.36306629	0.74509925
C	-0.00388501	-0.00041763	1.27050307
N	0.00386209	0.00028748	-1.23496570
C	-0.47823984	1.36323466	-0.79353373
C	-1.01522730	-1.02857737	0.73751890
C	-0.93743198	-1.09775326	-0.79554683
H	1.79775294	-1.20685704	-1.25066791
H	2.08531165	0.56151358	-1.13575660
H	-1.36154572	1.71201468	1.17786580
H	0.37307318	2.13772090	1.07185929
H	2.15834415	0.31887471	1.18848795
H	1.65969905	-1.39565954	1.07447531
H	-0.00734264	-0.00086023	2.38821307
H	0.15310560	2.15721295	-1.25463775
H	-1.52285695	1.52291570	-1.14707448
H	-0.80889282	-2.03222385	1.17890596
H	-2.04333745	-0.74239071	1.06308971
H	-1.93833383	-0.94942024	-1.26208635
H	-0.55141204	-2.08310478	-1.14452142

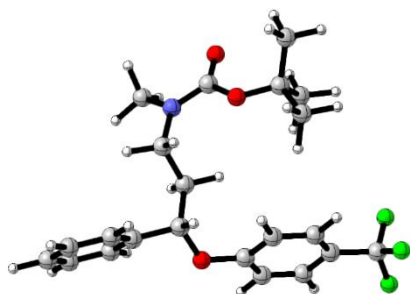
4-phenylbutan-1-ol



C	-2.87412900	0.59005500	-0.01765900
C	-2.20915900	0.27570200	-1.20737100
C	-1.02631600	-0.46943800	-1.17479200
C	-0.47837500	-0.90954800	0.04308900
C	-1.16425000	-0.59594500	1.22519400
C	-2.34900900	0.14648400	1.19925400
C	0.81158500	-1.70913700	0.06218100
C	2.04016900	-1.00308000	-0.55730800
C	2.69820300	0.09204700	0.30006200
C	1.82189100	1.30576300	0.63996800
O	1.26054400	1.93786400	-0.51095200
H	1.04491500	-2.00264800	1.09448300

H	1.02893700	1.02707600	1.34635200
H	-3.79145400	1.17224800	-0.04005900
H	-2.61099800	0.60797000	-2.16133300
H	-0.52417600	-0.71630700	-2.10809100
H	-0.76025000	-0.92956200	2.17888800
H	-2.85790100	0.38213000	2.13063200
H	0.64319500	-2.64403600	-0.49105700
H	2.80016700	-1.76860400	-0.76312600
H	1.76969300	-0.58054000	-1.53358800
H	3.05070900	-0.34645200	1.24681800
H	3.58864500	0.44996800	-0.23405100
H	2.43889000	2.06931300	1.12687600
H	0.47160900	1.43911500	-0.78083800

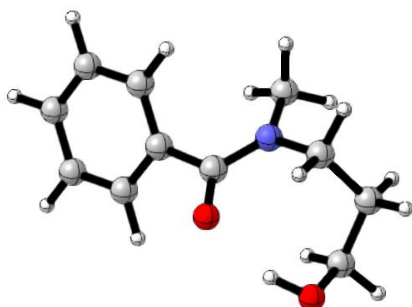
tert-butyl methyl(3-phenyl-3-(4-(trifluoromethyl)phenoxy)propyl)carbamate



C	-5.23731300	-1.94383200	1.46572600
C	-5.73299400	-2.52325400	0.36230200
C	-4.94522600	-2.68359300	-0.71132900
C	-3.67021500	-2.26622600	-0.67676900
C	-3.15756000	-1.68470900	0.42322600
C	-3.96102900	-1.52945500	1.49196600
C	-1.71168400	-1.20740800	0.44807200
O	-0.87056700	-2.26104400	0.03051500
C	-1.53946300	0.01839800	-0.45914900
C	0.49358100	-2.08882300	0.04418600
C	1.24169200	-2.73880600	-0.86820500
C	2.57425300	-2.60277200	-0.94272800
C	3.23200600	-1.76826400	-0.12052300
C	2.50300500	-1.12645300	0.80803900
C	1.16987500	-1.26918800	0.87356900
C	-2.40121400	1.21690800	-0.02727800
N	-2.09149100	2.37454300	-0.86487200
H	-1.45676700	-0.94566100	1.49986700
C	-2.89451300	2.52173300	-2.07397500
O	-0.30023600	2.97471000	0.53372500
C	1.00108100	3.44867700	0.70208500
C	1.54293200	2.73028900	1.94984200
C	1.89306100	3.07967600	-0.49055600
C	1.01300900	4.95775800	0.97639200
C	-1.04587400	3.22226400	-0.58445800
O	-0.77750000	4.11743600	-1.35099100
H	-3.65879700	1.72103800	-2.18357500
H	-3.42905100	3.49867400	-2.06243500
H	-2.24360600	2.47173400	-2.97632000
C	4.73720000	-1.64529000	-0.15776500
F	5.32856200	-2.72626400	-0.64186500
F	5.25506500	-1.40463600	1.03674600

F	5.07233400	-0.63023500	-0.93975400
H	-5.88080500	-1.80620300	2.35098100
H	-6.78150600	-2.86356600	0.33723100
H	-5.34680300	-3.15735500	-1.62287100
H	-3.04108500	-2.40541200	-1.57135500
H	-3.57782600	-1.05096600	2.40834800
H	-0.47301300	0.34263800	-0.46135300
H	-1.78211300	-0.24946700	-1.51433900
H	0.73901000	-3.41397400	-1.58230400
H	3.12574200	-3.17772000	-1.70476600
H	3.00187500	-0.45561600	1.52713500
H	0.64439300	-0.69347000	1.65102900
H	-3.48408900	0.96442000	-0.08737700
H	-2.21974300	1.45556700	1.04600100
H	0.92062400	2.95120000	2.84699800
H	1.54223900	1.62598200	1.81196900
H	2.58792000	3.03588800	2.18257800
H	1.82012400	1.99295300	-0.72572300
H	2.96141100	3.30141500	-0.26788400
H	1.64937800	3.64365700	-1.41616100
H	0.32239800	5.22189500	1.80933700
H	2.03316300	5.29808800	1.26590200
H	0.72249200	5.56807000	0.09503500

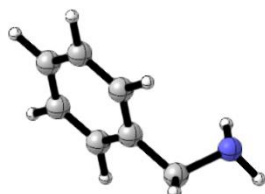
N-(3-hydroxypropyl)-N-methylbenzamide



N	-0.86241100	0.99402800	-0.12906300
C	-2.25123300	1.10054100	-0.60340200
C	-0.42183300	2.04558700	0.78433600
C	-3.30569400	0.62200900	0.40805100
C	-3.15745900	-0.84959600	0.81695100
O	-3.24752200	-1.73999600	-0.28248100
H	-2.20796100	-0.99241000	1.35887400
H	-0.21805300	2.98040800	0.24488800
C	-0.12326600	-0.10069900	-0.47741200
C	4.10925800	-0.31479800	0.26614900
C	3.26856600	-1.38318000	0.59791700
C	1.89557000	-1.29202100	0.36437800
C	1.34805100	-0.11900000	-0.17436700
C	2.19458900	0.94686100	-0.51160900
C	3.57154700	0.84615100	-0.29859600
O	-0.62597600	-1.07593700	-1.05900000
H	-2.42666900	2.15488100	-0.85249400
H	-2.33282200	0.52281500	-1.52611000
H	-1.21097000	2.23873300	1.51898900
H	0.47562700	1.74432700	1.32351200
H	-3.27974900	1.24803300	1.31227000

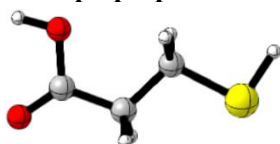
H	-4.29180600	0.76569500	-0.05247700
H	-3.96812100	-1.11411100	1.50547000
H	-2.38788100	-1.69990600	-0.74914300
H	5.17979300	-0.39031000	0.43844000
H	3.68437100	-2.29072600	1.02758500
H	1.23726100	-2.12703000	0.58485000
H	1.78020600	1.84710600	-0.95748300
H	4.22305300	1.67063800	-0.57625300

Amino-phenyl-methyl



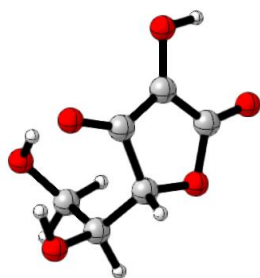
C	1.61807200	-1.10479400	0.11039000
C	2.19384200	0.10363900	0.20624200
C	1.45140700	1.21067800	0.05053800
C	0.13700900	1.10738700	-0.20039400
C	-0.44617800	-0.09945100	-0.29826200
C	0.30330800	-1.20285300	-0.14072700
C	-1.91702400	-0.23474100	-0.57549200
N	-2.68490900	0.17542400	0.60623900
H	-2.23301200	0.33324800	-1.47921400
H	2.22493100	-2.01673800	0.23854400
H	3.27396100	0.18661900	0.41297400
H	1.92158800	2.20520400	0.12959400
H	-0.46836300	2.02024700	-0.32616200
H	-0.16809300	-2.19657000	-0.21803100
H	-3.60305400	-0.30077900	0.62217800
H	-2.19621600	-0.13838500	1.46267800

3-mercaptopropanoic acid



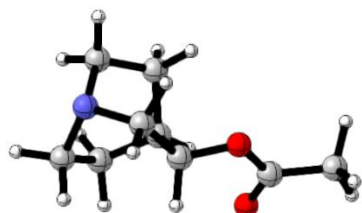
C	-1.66696100	-0.16038000	0.00013000
C	-0.21011500	-0.59372500	0.00121600
C	0.83505300	0.53492500	-0.00112200
O	-2.62288400	-0.89897900	-0.00113600
O	-1.81965900	1.17765000	0.00079600
S	2.50634800	-0.19616200	0.00016400
H	3.18065200	0.96825700	-0.00198200
H	-0.07084000	-1.23575900	0.90395000
H	-0.07055900	-1.23951100	-0.89874600
H	0.71076100	1.17542200	-0.90545200
H	0.71103200	1.17885600	0.90084500
H	-2.77013400	1.37704900	0.00014900

Ascorbate



O	0.57268800	1.77008100	-0.82857600
C	-0.20780600	0.77816600	-0.64013200
C	0.28895700	-0.65472800	-0.85865700
C	1.64679100	-0.91363400	-0.17910700
O	2.66434800	-0.27280300	-0.94402600
C	1.69087300	-0.50805100	1.31042300
O	1.88087800	0.87915600	1.55871900
O	-0.73419800	-1.53274200	-0.34690100
C	-1.81077400	-0.73917700	0.03465200
O	-2.84431700	-1.23298500	0.49201800
C	-1.49744300	0.63957700	-0.16277200
O	-2.39156800	1.62821400	0.20690900
H	-3.15760900	1.15338400	0.57754400
H	0.40946800	-0.86259600	-1.92987800
H	1.84524700	-1.99234300	-0.23278400
H	2.37904600	0.66144700	-1.02792500
H	0.76820700	-0.87549700	1.79028400
H	2.54362700	-1.01190000	1.78147300
H	1.36578500	1.40322500	0.90969100

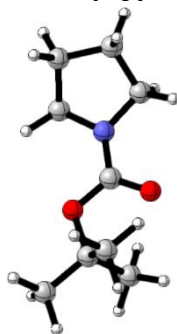
Tertiary amine HAT catalyst



C	-2.34157900	0.91521900	-0.74564800
N	-2.19865400	-0.57064400	-0.59775100
C	-0.87376000	-0.98287300	-1.16765300
C	-1.44727800	1.46977700	0.35531400
C	0.22999500	-0.03874300	-0.69175200
C	-0.31271700	0.49123000	0.62884800
C	-2.21745900	-0.91004000	0.86319500
C	-0.83415300	-0.66942500	1.46575000
O	1.43411600	-0.73038800	-0.49887700
O	2.12548200	1.28580300	0.06925100
C	2.38373300	0.11564200	-0.08308600
C	3.77711200	-0.39205800	0.19567900
H	-3.39856200	1.22966800	-0.59509700
H	-2.05879300	1.27938000	-1.75866700
H	-0.92780800	-0.95203400	-2.27890200
H	-0.63861600	-2.01471900	-0.82322600
H	-1.02389800	2.44699100	0.03187800
H	-2.04556600	1.61286100	1.28281000
H	0.46193900	0.76681300	-1.42388700

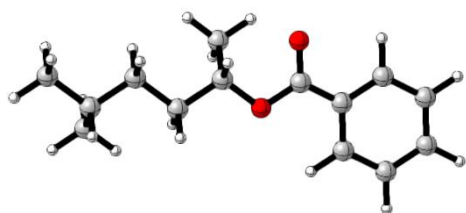
H	0.50078800	1.01154200	1.18222400
H	-2.49486200	-1.98032100	0.99038900
H	-2.96257200	-0.26600200	1.38179000
H	-0.18587700	-1.56757700	1.35685100
H	-0.85463600	-0.45733900	2.55815600
H	4.42058200	0.45272800	0.52891800
H	3.73675700	-1.16493500	0.99559500
H	4.20154500	-0.83824400	-0.73144800

tert-butyl pyrrolidine-1-carboxylate



N	1.28665800	-0.09482300	-0.29500300
C	1.94409500	1.19202500	-0.50449400
C	3.20389500	1.09602900	0.33851000
C	3.48510600	-0.39665300	0.46396100
C	2.36723800	-1.07681500	-0.30757200
O	-0.91660700	0.69075700	-0.13900900
C	-2.22061400	0.21337400	0.05426500
C	-2.57439800	-0.76191800	-1.06073400
C	-2.30609600	-0.49764600	1.39831400
C	-3.19767600	1.38147700	0.03557000
C	-0.05114100	-0.32951800	-0.12405200
O	-0.45038800	-1.45770000	0.04028300
H	1.29751200	2.02850700	-0.15670600
H	4.05132800	1.61180700	-0.16605100
H	-3.46065700	-0.38374600	-1.61786000
H	2.15823700	1.39677600	-1.57736500
H	3.07885900	1.58180100	1.33210800
H	3.46781000	-0.70854200	1.53221800
H	4.48941300	-0.66640000	0.06734000
H	2.68569500	-1.30185500	-1.35001700
H	2.06792000	-2.05167900	0.13853400
H	-1.71168500	-0.85677000	-1.75757700
H	-2.80921600	-1.75749700	-0.62198800
H	-1.59246700	-1.35154300	1.41301400
H	-3.34117100	-0.87718900	1.55147800
H	-2.04749700	0.21583900	2.21237500
H	-3.13595100	1.90179000	-0.94634900
H	-4.23248100	1.00138400	0.18908500
H	-2.93875300	2.09449600	0.84998800

5-methylhexan-2-yl benzoate



C	-4.53251700	0.57230000	-0.37663000
C	-3.34338900	-0.37783700	-0.32262100
C	-5.82449800	-0.23249300	-0.42565200
C	-4.53226200	1.45557400	0.86413900
C	-2.05138100	0.42705300	-0.27359900
C	-0.86225300	-0.52308400	-0.21959000
C	-0.96499300	-1.39355500	1.02596700
H	-4.45744400	1.20910700	-1.28638300
H	-0.86256800	-1.16918300	-1.12590700
O	0.32710700	0.21775500	-0.17448300
C	1.37749200	-0.60964100	-0.12685800
C	5.21905000	0.92815100	0.02359400
C	4.12405300	1.79070500	-0.02610900
C	2.82995200	1.27264000	-0.07674700
C	2.63094900	-0.10790300	-0.07780100
C	3.72592600	-0.97045000	-0.02819600
C	5.02004700	-0.45239100	0.02254000
O	1.20510900	-1.80530400	-0.12775600
H	-3.34359800	-1.02323600	-1.22932300
H	-3.41852800	-1.01452100	0.58715400
H	-6.69349600	0.46185900	-0.46507400
H	-5.82463900	-0.87801500	-1.33237600
H	-5.89963700	-0.86917800	0.48412400
H	-5.40089100	2.15043800	0.82569700
H	-3.58837700	2.04427400	0.89962600
H	-4.60739200	0.81795700	1.77323500
H	-2.05126600	1.07247900	0.63312500
H	-1.97633600	1.06376400	-1.18335200
H	-0.09643400	-2.08831100	1.06627600
H	-1.90890200	-1.98213900	0.98977500
H	-0.96469600	-0.74651000	1.93153200
H	6.23952900	1.33666100	0.06363300
H	4.28099900	2.87946700	-0.02535100
H	1.96634000	1.95280900	-0.11581200
H	3.56895800	-2.05920500	-0.02905000
H	5.88358600	-1.13254100	0.06172500

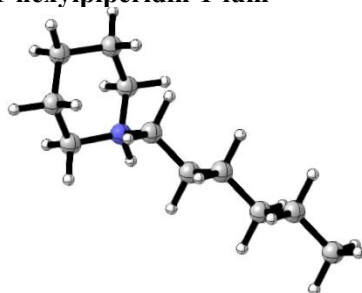
Aminium radical cation



C	0.02657200	0.76944000	1.24437500
C	0.02657200	-0.77042400	1.21390200
N	0.71832100	-1.24903500	0.00000000
C	0.02657200	-0.77042400	-1.21390200
C	0.02657200	0.76944000	-1.24437500
C	-0.70051600	1.29253500	0.00000000

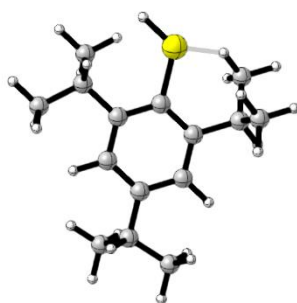
H	0.72186600	-2.24902900	0.00000000
H	-0.47480600	1.11324200	2.12489700
H	1.03516700	1.12669000	1.24733600
H	0.53412600	-1.14052500	2.08010900
H	-0.98238500	-1.12665100	1.21101800
H	0.53412600	-1.14052500	-2.08010900
H	-0.98238500	-1.12665100	-1.21101800
H	-0.47480600	1.11324200	-2.12489700
H	1.03516700	1.12669000	-1.24733600
H	-0.69788400	2.36253200	0.00000000
H	-1.71106300	0.94083100	0.00000000

1-hexylpiperidin-1-ium



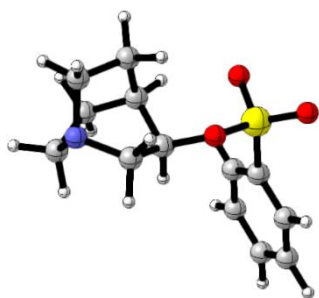
C	2.98124700	1.33334100	-0.49975200
C	2.42428100	1.16476700	0.90542100
N	1.63635800	-0.10241300	0.97354200
C	2.42197500	-1.32349100	0.62306200
C	2.97896700	-1.17397200	-0.78426300
C	3.78801900	0.11231600	-0.93613600
H	1.27485800	-0.21265400	1.94783700
C	0.53664500	0.01359400	-0.03991100
C	-0.81241100	-0.06494100	0.66250600
C	-1.92896000	0.05294400	-0.36651300
C	-3.27801600	-0.02559100	0.33590400
C	-4.39462800	0.09223500	-0.69316400
C	-5.74375400	0.01371900	0.00932200
H	3.64225100	2.22851100	-0.52058500
H	2.12535200	1.45340900	-1.20091100
H	3.26357100	1.12026600	1.63517900
H	1.76625900	2.02769400	1.15273900
H	1.75979300	-2.21700600	0.66777900
H	3.25958700	-1.44899400	1.34516900
H	3.63842300	-2.04298100	-1.00524700
H	2.12303800	-1.13236100	-1.49442300
H	4.70347400	0.04013700	-0.30720700
H	4.05422000	0.23387100	-2.00993900
H	0.62236300	0.98869200	-0.56961200
H	0.62081000	-0.81769400	-0.77517700
H	-0.89812900	-1.04003900	1.19220800
H	-1.84331200	1.02806100	-0.89614600
H	-1.84485900	-0.77840300	-1.10182800
H	-3.36373400	-1.00068900	0.86560500
H	-3.36225000	0.80571600	1.07123900
H	-4.30898000	1.06735200	-1.22279700
H	-4.31046300	-0.73905300	-1.42843100
H	-6.55971000	0.09986000	-0.74269700
H	-5.82940200	-0.96139800	0.53895400
H	-5.82785500	0.84506600	0.74463700

2,4,6-triisopropylbenzenethiol



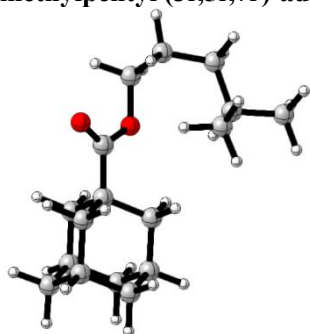
C	-0.96162200	0.02839600	-0.08384600
C	-0.35050800	-1.21737600	0.05786400
C	1.03957900	-1.32183500	0.00889100
C	1.81842800	-0.18056700	-0.18190500
C	1.20732800	1.06517500	-0.32370900
C	-0.18277400	1.16966400	-0.27464100
S	-2.77043800	0.16441600	-0.02003200
C	-0.83878600	2.50670300	-0.42681700
C	0.22727600	3.57683000	-0.62096900
C	-1.64877000	2.81912500	0.82447400
C	3.31019200	-0.29276300	-0.23458000
C	3.71722800	-1.74927200	-0.05473500
C	3.92128300	0.54563900	0.88052900
C	-1.18650900	-2.44230500	0.26249100
C	-1.53498600	-3.05156700	-1.08913400
C	-2.46796900	-2.06507300	0.99403500
H	-3.35975400	1.36558200	-0.15667500
H	1.52155900	-2.30434000	0.12069100
H	1.82153200	1.96511000	-0.47428100
H	-1.51328700	2.49021100	-1.31200600
H	0.81992200	3.34933500	-1.53521200
H	-0.26135100	4.57035700	-0.73394400
H	0.90215200	3.59279600	0.26391700
H	-2.42829100	2.03765700	0.96738700
H	-2.13702200	3.81293000	0.71115000
H	-0.97337900	2.83538400	1.70902900
H	3.67530800	0.07541900	-1.21933600
H	3.27123700	-2.36295700	-0.86919700
H	4.82647700	-1.83157100	-0.09397800
H	3.35159100	-2.11770400	0.92980700
H	3.62444900	1.61036000	0.75003600
H	5.03047300	0.46280300	0.84102300
H	3.55558700	0.17667100	1.86480800
H	-0.61720400	-3.18296600	0.86741800
H	-0.59916800	-3.32762200	-1.62464800
H	-2.15644700	-3.96212800	-0.93588100
H	-2.10370300	-2.31067400	-1.69436200
H	-2.21436000	-1.61966900	1.98203800
H	-3.08912800	-2.97586100	1.14677100
H	-3.03652400	-1.32442100	0.38827300

Quinuclidine sulfonate catalyst



C	-2.92596000	-2.07309100	0.14217600
N	-3.39215600	-0.90299700	0.95676300
C	-2.19830400	-0.26147600	1.59959500
C	-2.32905000	-1.42584400	-1.10049500
C	-1.06366600	-0.10833100	0.58718700
C	-1.79585800	-0.04378200	-0.74679300
C	-4.03442800	0.09389800	0.03820500
C	-2.95656100	0.93662000	-0.64191900
O	-0.33826400	1.06868100	0.81963800
S	0.94879500	1.45646000	-0.15431200
O	1.52880800	2.71017600	0.28636700
O	0.49396400	1.59042400	-1.52466400
C	2.18149800	0.16215500	-0.05714200
C	2.31816500	-0.75072000	-1.10287300
C	3.27860800	-1.75927200	-1.02700600
C	4.10251000	-1.85491300	0.09438500
C	3.96595200	-0.94198000	1.14004900
C	3.00529400	0.06659700	1.06429700
H	-3.77898500	-2.73591600	-0.12572400
H	-2.20024500	-2.71838200	0.68608600
H	-1.85152200	-0.89765200	2.44444400
H	-2.48772600	0.74677800	1.97181700
H	-1.49651600	-2.05735900	-1.48374900
H	-3.11450000	-1.33145400	-1.88340800
H	-0.31865500	-0.93365300	0.63742200
H	-1.09289800	0.29680100	-1.53973600
H	-4.70680800	0.75822400	0.62593100
H	-4.62435000	-0.44518600	-0.73635700
H	-2.68351900	1.81878500	-0.02056300
H	-3.27325300	1.35883500	-1.62181300
H	1.66849400	-0.67516200	-1.98727600
H	3.38638400	-2.47932200	-1.85166200
H	4.85995600	-2.65030000	0.15417200
H	4.61572700	-1.01740000	2.02444400
H	2.89752400	0.78656700	1.88889300

4-methylpentyl (3r,5r,7r)-adamantane-1-carboxylate



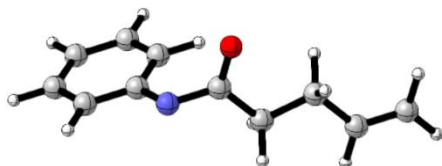
C	-3.06089900	0.27539800	-1.29636700
C	-2.76562400	1.71693800	-0.84143500
C	-2.02546900	1.68664900	0.50867200
C	-2.90476500	0.98580600	1.56179700
C	-3.20246800	-0.45568800	1.10742000
C	-3.94115200	-0.42553000	-0.24389700
C	-1.73879400	-0.49677600	-1.45435100
C	-0.70022700	0.91763700	0.35561700
C	-1.87914600	-1.22792500	0.95376800
C	-0.98246600	-0.53155700	-0.10930200
C	0.29318300	-1.34835400	-0.25523600
O	1.14881200	-1.14153800	0.77092700
O	0.51780400	-2.13457800	-1.15627100
C	2.36207500	-1.93572300	0.79098200
C	3.45643700	-1.41286000	-0.13438000
C	4.05647700	-0.04986000	0.24329000
C	3.15009800	1.18482800	0.07327400
C	3.89296600	2.44484700	0.53813400
C	2.66764400	1.35172100	-1.37402100
H	-3.82371200	-0.96044100	1.85903500
H	-1.92788300	-1.52015300	-1.79581900
H	2.68004500	-1.89537400	1.83688700
H	2.27006800	1.05546600	0.71368700
H	-3.58322600	0.29166400	-2.26175100
H	-2.15340700	2.23157800	-1.59505300
H	-3.70247600	2.28291500	-0.74518800
H	-1.80621900	2.71201800	0.83446700
H	-3.84462800	1.53866400	1.69605000
H	-2.39326500	0.97703200	2.53434100
H	-4.17414200	-1.44880500	-0.56920400
H	-4.89725800	0.10514900	-0.13699700
H	-1.10808200	-0.02177800	-2.21687400
H	-0.05676400	1.42033200	-0.37683400
H	-0.15929000	0.90476300	1.30751400
H	-2.07769400	-2.26212400	0.64271500
H	-1.34757900	-1.26760800	1.91246400
H	2.10013600	-2.96445100	0.52884100
H	4.25928700	-2.16350000	-0.10246600
H	3.08570300	-1.41292800	-1.16401000
H	4.40055000	-0.09273500	1.28782100
H	4.95952300	0.10527000	-0.36637200
H	3.25186600	3.33206900	0.46711900
H	4.22437100	2.35195000	1.57995000
H	4.78257700	2.62602300	-0.08053400
H	2.06852600	2.26407100	-1.48240600
H	2.05152200	0.51035300	-1.70733500
H	3.52129200	1.43219600	-2.06108200

5-methyl-1-phenylpyrrolidin-2-one



N	0.61456000	-0.05773500	-0.20798500
C	1.47919700	1.09845500	-0.42609800
C	2.68527400	0.81934400	0.45409600
C	2.71441200	-0.69558400	0.61909100
C	1.51923300	-1.20326900	-0.16913000
O	1.35546000	-2.29874100	-0.65119300
C	0.78299800	2.38413000	0.00019700
C	-0.64496000	-0.06536000	-0.08037700
C	-1.31791000	-1.26989000	0.12391300
C	-2.70566100	-1.27828700	0.26437700
C	-3.42033300	-0.08217400	0.20066200
C	-2.74739400	1.12235200	-0.00352900
C	-1.35963300	1.13075300	-0.14409100
H	1.75021900	1.23787400	-1.49657600
H	3.61792600	1.17650900	-0.03714900
H	2.61742400	1.34427300	1.43311500
H	2.62004400	-0.97295800	1.69285300
H	3.67026600	-1.13597400	0.25690600
H	1.46062600	3.24943400	-0.17536100
H	-0.14812700	2.51616900	-0.59511000
H	-0.75427700	-2.21319400	0.17423500
H	-3.23639900	-2.22826900	0.42536000
H	-4.51471400	-0.08885800	0.31142400
H	-3.31103600	2.06565000	-0.05375100
H	-0.82889900	2.08060000	-0.30518300

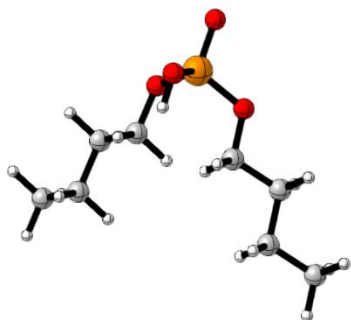
1-(phenyl- λ^2 -azaneyl)pent-4-en-1-one



N	-0.58633300	-1.38383800	-0.23099700
C	0.63741700	-1.03665700	0.27498900
C	1.64023800	-0.32336700	-0.59840800
O	0.91448200	-1.30131500	1.42055900
C	2.90908600	-0.05440000	0.19979900
C	3.90391500	0.65318800	-0.66648600
C	5.09899500	0.99225400	-0.17236200
C	-1.61993900	-0.52821900	-0.13800400
C	-1.44492700	0.71284700	0.47405400
C	-2.51686500	1.60013100	0.57064400
C	-3.76367200	1.24634700	0.05507600
C	-3.93866600	0.00534300	-0.55705800
C	-2.86674600	-0.88200300	-0.65357100
H	1.88398300	-0.95975800	-1.47836200
H	1.20896100	0.64211900	-0.94571700
H	2.66532300	0.58192900	1.07983000

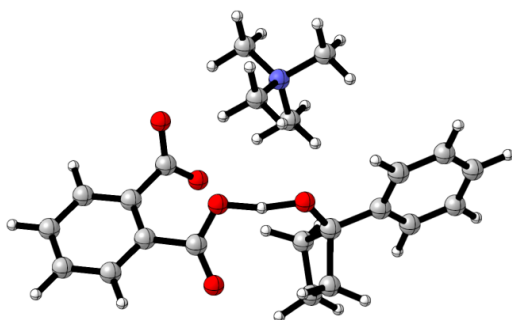
H	3.34031300	-1.01987000	0.54724000
H	3.65157500	0.89420300	-1.70975400
H	5.83004200	1.51226100	-0.80898400
H	5.35135300	0.75130100	0.87082900
H	-0.46161600	0.99188700	0.88059000
H	-2.37887000	2.57885700	1.05346800
H	-4.60897000	1.94609400	0.13128900
H	-4.92195900	-0.27363600	-0.96367000
H	-3.00466500	-1.86077700	-1.13628600

Dibutyl hydrogen phosphate



P	0.00000100	-2.04413700	-0.06263800
O	0.00034700	-3.33567900	-0.78535300
O	0.00025800	-2.31710400	1.52916000
H	0.00002000	-1.46144900	1.92316500
O	1.31908500	-1.20323200	-0.46405200
C	4.17913400	2.73444100	-0.15175300
C	2.89349900	2.07431500	0.32880800
C	2.74317400	0.71140300	-0.33422000
C	1.45744000	0.05132500	0.14625400
O	-1.31901500	-1.20317800	-0.46418000
C	-4.17936700	2.73412600	-0.15170400
C	-2.89370100	2.07397300	0.32890600
C	-2.74322600	0.71125700	-0.33432900
C	-1.45756000	0.05119100	0.14633000
H	4.28896000	3.73039000	0.33275800
H	5.04797100	2.09332100	0.11812100
H	4.13997600	2.86184100	-1.25673500
H	2.02456200	2.71543500	0.05893400
H	2.93255700	1.94682800	1.43374200
H	3.61201200	0.07033100	-0.06443300
H	2.70401700	0.83893900	-1.43924100
H	0.58860200	0.69253300	-0.12357100
H	1.49659700	-0.07607500	1.25123700
H	-4.28934100	3.72995400	0.33291800
H	-4.13932500	2.86222200	-1.25666300
H	-5.04842900	2.09281200	0.11707200
H	-2.93374300	1.94592600	1.43377800
H	-2.02463800	2.71528700	0.06013000
H	-2.70318400	0.83944000	-1.43923900
H	-3.61228900	0.07003000	-0.06550400
H	-1.49760200	-0.07685600	1.25120200
H	-0.58849800	0.69250500	-0.12244600

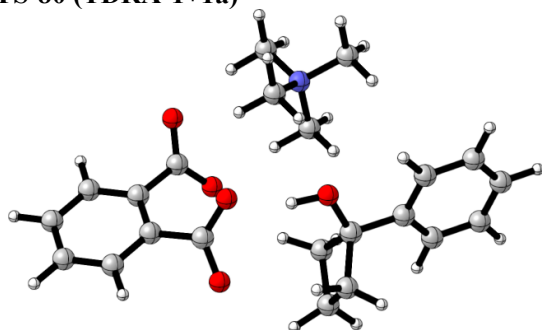
IBO Analyses and Spin Population Analyses TS (TDRA-1+1a)



C	-5.93978800	-0.34108200	0.16035700
C	-5.17996800	0.11431100	-0.92221500
C	-3.83312000	-0.24088100	-1.03709500
C	-3.21390900	-1.05444400	-0.07330400
C	-3.99371300	-1.51875300	1.00024400
C	-5.33979700	-1.16493600	1.11859200
C	-1.74755000	-1.42617700	-0.22122600
H	-6.98804100	-0.06781600	0.25073700
H	-5.64110000	0.73644900	-1.68652400
H	-3.24459300	0.09237400	-1.88601600
H	-5.92087800	-1.53424500	1.96012300
C	-0.94665200	-1.53261500	1.17719100
C	-0.94799000	-3.07372200	1.11203800
C	-1.48870300	-3.00718800	-0.33130600
H	0.03621100	-3.53617800	1.20845200
H	-1.63913800	-3.54227500	1.82130300
H	-2.39307300	-3.58002500	-0.56066400
H	-0.71064700	-3.17481700	-1.07699300
H	-1.47416200	-1.06776200	2.01730000
H	0.04151700	-1.08291600	1.07617500
O	-1.15308900	-0.67086100	-1.18755800
H	0.04626900	-0.65381700	-1.17407100
H	-3.55093400	-2.16378900	1.75411600
C	5.78114300	-1.39561900	-0.41095200
C	6.04104300	-0.18847500	0.25630600
C	4.98512100	0.63928800	0.62709500
C	3.65895800	0.27968000	0.32798500
C	3.39829200	-0.93007200	-0.35681900
C	4.46781100	-1.76091200	-0.70864500
C	2.00364300	-1.35106300	-0.74563200
O	1.68414000	-2.54309400	-0.73117300
O	1.22873100	-0.36162500	-1.09114400
C	2.56246800	1.17286600	0.82371000
O	2.51523000	2.37235400	0.43928200
O	1.74342400	0.70268100	1.66509800
H	6.60298500	-2.04786000	-0.69523100
H	7.06371800	0.09799100	0.48778000
H	5.17078700	1.57234100	1.15157200
H	4.24824900	-2.69489900	-1.21701300
N	-0.96391800	2.96634000	-0.16277100
C	-2.33403200	3.43354600	-0.55405900
H	-2.90896600	2.57452900	-0.90595600
H	-2.82293500	3.87189000	0.31871600
H	-2.24393400	4.18059300	-1.34575400
C	-1.09307300	1.91650500	0.91554100
H	-1.58316100	2.37478300	1.77805800

H	-1.69798000	1.10338000	0.52124300
H	-0.09832600	1.55587300	1.18653100
C	-0.14675100	4.11744200	0.36123400
H	-0.06932800	4.87431700	-0.42295700
H	-0.65237100	4.53415900	1.23546800
H	0.84340200	3.73561200	0.62356900
C	-0.27201300	2.37391200	-1.37078000
H	-0.21128400	3.14999100	-2.13752800
H	0.72313500	2.04399600	-1.07602500
H	-0.85400000	1.51844200	-1.71260700

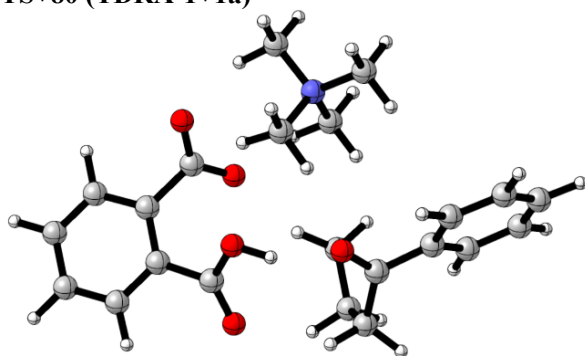
TS-80 (TDRA-1+1a)



C	6.09896200	0.25886700	-0.16564000
C	5.31583100	0.69844900	0.90291300
C	4.01206900	0.22334500	1.06553700
C	3.45887700	-0.69630100	0.16019400
C	4.26119000	-1.13671600	-0.90382800
C	5.56524300	-0.66676800	-1.06512700
C	2.03335400	-1.19294600	0.34463200
H	7.11370500	0.62673900	-0.29329500
H	5.72294300	1.40740200	1.62053600
H	3.41086000	0.54998700	1.90643600
H	6.16418600	-1.02322900	-1.89949900
C	1.25273200	-1.45509900	-0.99452700
C	1.42646100	-2.98294800	-0.79682700
C	1.91057300	-2.72704600	0.65379400
H	0.51100800	-3.57122900	-0.88689700
H	2.19757600	-3.42036500	-1.44000200
H	2.82158400	-3.23326200	0.98845400
H	1.10921300	-2.89076400	1.37940300
H	1.68009100	-1.01362800	-1.90207700
H	0.21288300	-1.13402800	-0.91242100
O	1.41260500	-0.33302800	1.27913400
H	0.44938200	-0.55265600	1.33372200
H	3.86769300	-1.85305100	-1.61864700
C	-5.66259400	-1.87810100	0.39063000
C	-6.02281800	-0.72735100	-0.33314700
C	-5.05119800	0.18806900	-0.72147700
C	-3.70552300	-0.03000100	-0.39686700
C	-3.34479700	-1.17823000	0.35164000
C	-4.33347900	-2.10156200	0.72660500
C	-1.93417000	-1.39156300	0.81373100
O	-1.48383100	-2.56619800	0.72715600
O	-1.28637600	-0.41878400	1.27843800
C	-2.66090100	0.91670800	-0.90771000
O	-2.77996900	2.14601800	-0.67641500

O	-1.72422100	0.41099000	-1.58451200
H	-6.42678200	-2.58903000	0.69232100
H	-7.06470400	-0.55409400	-0.58881600
H	-5.31481300	1.07784800	-1.28521100
H	-4.03635100	-2.98024200	1.28995200
N	0.67194000	3.02993700	-0.05755000
C	1.97479000	3.65500000	0.34283400
H	2.62325200	2.87634400	0.75030600
H	2.44068000	4.09884700	-0.53941500
H	1.78589900	4.42616700	1.09261500
C	0.94928600	1.92993600	-1.05560500
H	1.44742200	2.37739200	-1.91878900
H	1.59259500	1.19980200	-0.57216100
H	0.00327300	1.46499800	-1.34560800
C	-0.23796200	4.05036700	-0.68546800
H	-0.40780800	4.85480400	0.03397000
H	0.24728100	4.44584100	-1.58059000
H	-1.18008200	3.55108400	-0.93101800
C	0.00026800	2.45364800	1.16912800
H	-0.16907000	3.27272000	1.87193300
H	-0.94437800	2.00189700	0.87292500
H	0.65721500	1.69213300	1.58516500

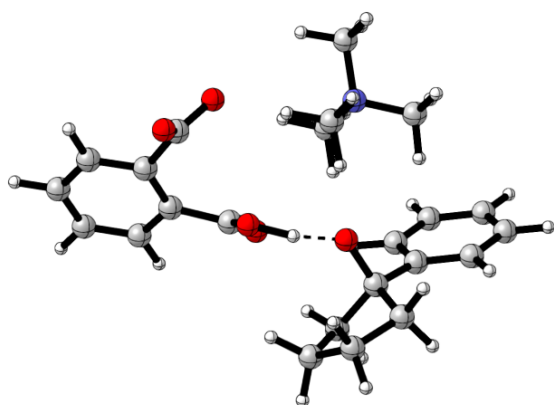
TS+80 (TDRA-1+1a)



C	6.04413500	0.29091800	-0.18814400
C	5.28610400	0.80239400	0.86817100
C	4.00202400	0.31786300	1.09338800
C	3.47267000	-0.70791000	0.29513100
C	4.23411800	-1.21284000	-0.76976800
C	5.50910800	-0.70030900	-1.01659200
C	2.14466600	-1.24440000	0.72731200
H	7.05009800	0.66134200	-0.36527200
H	5.70125500	1.56590500	1.52054000
H	3.40657700	0.68630500	1.92238400
H	6.09400500	-1.08719600	-1.84625500
C	0.92200800	-1.53238800	-1.52037700
C	1.22970100	-2.87381900	-0.92640300
C	1.79418100	-2.70422500	0.52547100
H	0.31596300	-3.47178100	-0.85722400
H	1.95219200	-3.42116400	-1.54365400
H	2.67294200	-3.33560400	0.69849100
H	1.01207400	-2.94707300	1.24613700
H	1.60420200	-1.07986400	-2.23480300
H	-0.02307200	-1.03036900	-1.33736000
O	1.38881600	-0.48413400	1.33895800

H	-0.33910100	-0.61947700	1.45469000
H	3.83432200	-1.99934800	-1.40159200
C	-5.61619000	-1.86645700	0.37357100
C	-5.94287700	-0.70499500	-0.33226700
C	-4.94428800	0.19718100	-0.70429000
C	-3.60314400	-0.04066000	-0.38755800
C	-3.28750000	-1.19994000	0.34731600
C	-4.28622500	-2.11147500	0.70879400
C	-1.90436600	-1.48181100	0.81761700
O	-1.39566700	-2.59341200	0.85152800
O	-1.28318400	-0.38594000	1.28160000
C	-2.52139400	0.91098500	-0.89577800
O	-2.66631600	2.13148900	-0.61112600
O	-1.58633800	0.38082300	-1.55285200
H	-6.39119600	-2.57080800	0.66401200
H	-6.97873600	-0.50261000	-0.59459000
H	-5.19260600	1.10274400	-1.25015900
H	-4.00395000	-2.99983000	1.26640400
N	0.64741400	3.06747300	-0.08536000
C	1.94174100	3.71737700	0.29209900
H	2.60609100	2.95845200	0.71107500
H	2.39543800	4.15030900	-0.60187100
H	1.75057400	4.50126200	1.02826300
C	0.91503200	1.96528600	-1.08511000
H	1.39967600	2.41608300	-1.95488700
H	1.57891700	1.23915200	-0.61604800
H	-0.03872600	1.48256000	-1.36075300
C	-0.29690800	4.06841800	-0.70299500
H	-0.46717700	4.87092000	0.01905600
H	0.16888700	4.46924800	-1.60623000
H	-1.23263000	3.53166800	-0.92218500
C	-0.00637000	2.48521300	1.14668400
H	-0.11935500	3.28942100	1.87783100
H	-0.98191500	2.09040200	0.85908600
H	0.63552000	1.69396100	1.53078700

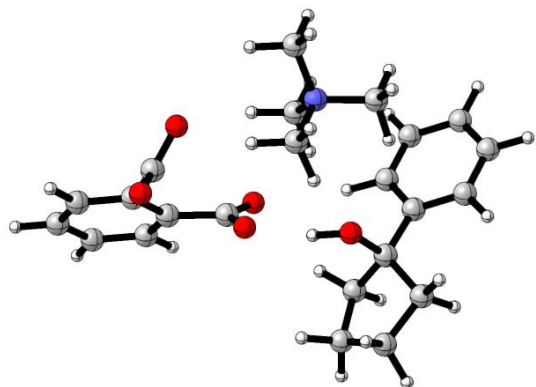
TS (TDRA-1+1e)



C	-5.54356118	1.77954365	1.16964885
C	-4.57281418	2.69838165	1.58879285
C	-3.21706218	2.43016465	1.38068385
C	-2.81060318	1.25246465	0.74747885
C	-3.78818218	0.31077065	0.35125685
C	-5.15140118	0.59120265	0.55778785

C	-3.44003818	-1.04107235	-0.18683415
O	-2.76089718	-1.85140435	0.49308185
O	-3.91461318	-1.36918235	-1.31261015
C	-1.33943818	1.07104365	0.47549685
O	-0.49267018	1.41784965	1.30161885
O	-1.09291518	0.56549765	-0.70502315
H	-6.59843118	1.98710865	1.32765385
H	-4.87197418	3.62321765	2.07508485
H	-2.45489918	3.13382765	1.70160685
H	-5.89099118	-0.13854335	0.24146685
C	1.82108482	2.39050665	-1.05415915
C	2.29843082	0.92246965	-1.22989815
C	2.87325682	0.98134665	-2.67508815
C	1.83541782	1.81041665	-3.45849515
C	1.16712282	2.74795765	-2.40694815
H	1.14282982	2.49446965	-0.20392915
H	2.69977482	3.02094065	-0.86368915
H	3.84419682	1.49526665	-2.64865415
H	3.02410882	-0.02127535	-3.08871615
H	2.30553182	2.36707565	-4.27747615
H	1.08702582	1.14792365	-3.90494815
H	1.30562582	3.80814065	-2.64805915
H	0.08835482	2.56613965	-2.36741615
C	3.27680882	0.45505065	-0.15170515
C	2.91389482	0.61092265	1.19895285
C	4.47027982	-0.21975535	-0.44529615
C	3.72271182	0.10985065	2.22051785
H	1.97932582	1.10883765	1.44379785
C	5.28137682	-0.72849235	0.57714585
H	4.77494282	-0.35885135	-1.47853615
C	4.91056582	-0.56689735	1.91496285
H	3.42603082	0.24873965	3.25792785
H	6.20467882	-1.24583735	0.32570185
H	5.54226382	-0.95525635	2.71039185
O	1.22083782	0.02435765	-1.22899315
H	0.00701282	0.42477965	-0.93997715
N	0.51804482	-2.93031535	0.34823285
C	-0.10087818	-4.14371235	0.97494485
C	-0.09948118	-2.71431035	-1.01853715
C	0.26626282	-1.73481135	1.24022985
C	2.00229882	-3.10367135	0.19104285
H	0.09586982	-5.01217135	0.34202785
H	0.33735782	-4.29582535	1.96394085
H	0.38504982	-1.84959035	-1.47172615
H	-1.16637718	-2.53735335	-0.88650315
H	0.71133882	-0.86435535	0.76667085
H	-0.80946318	-1.60658235	1.34576985
H	2.19180782	-3.96506735	-0.45374415
H	2.44904282	-3.26212135	1.17476185
H	-1.17578718	-3.97107935	1.05782185
H	0.07616282	-3.61857135	-1.60716015
H	2.40370382	-2.19261435	-0.25516115
H	0.74069182	-1.92908435	2.20473785

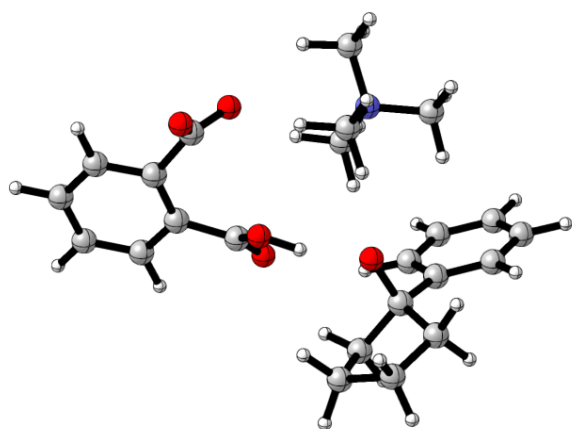
TS-71 (TDRA-1+1e)



C	-5.56910500	1.79300400	1.23317600
C	-4.57508800	2.72514600	1.58049500
C	-3.22699600	2.43833400	1.35931000
C	-2.84122400	1.23080600	0.77008700
C	-3.84316000	0.28046500	0.44829300
C	-5.20490900	0.57666900	0.67049200
C	-3.50941400	-1.08222900	-0.05641900
O	-2.87808400	-1.92843000	0.60657100
O	-3.98905000	-1.35969300	-1.20382000
C	-1.37780900	0.99001500	0.44873100
O	-0.52947700	1.37679100	1.28670200
O	-1.14455000	0.41782700	-0.65794700
H	-6.61666000	2.02012200	1.41062500
H	-4.85902900	3.67721700	2.02186200
H	-2.45104700	3.14724400	1.63184700
H	-5.95613600	-0.16407100	0.41228600
C	1.80607700	2.35957400	-1.10564100
C	2.41893400	0.95939200	-1.32016300
C	3.11477400	1.12716500	-2.68269600
C	2.10547200	1.93999900	-3.52437200
C	1.26839500	2.76251200	-2.49736300
H	1.03840500	2.36232400	-0.32719900
H	2.60814500	3.03657700	-0.78410600
H	4.04971000	1.68723200	-2.54801700
H	3.35916700	0.16001900	-3.13513000
H	2.61475300	2.57704800	-4.25605600
H	1.45449200	1.26090200	-4.08330000
H	1.35553100	3.84273500	-2.65960900
H	0.20623400	2.50980900	-2.57913100
C	3.30117400	0.47452200	-0.17289000
C	2.85871700	0.62030900	1.15374500
C	4.50648500	-0.20558800	-0.40013900
C	3.60045400	0.09892500	2.21643400
H	1.91457700	1.12083400	1.35342100
C	5.25113900	-0.73176800	0.66272100
H	4.87310100	-0.33333600	-1.41449000
C	4.80010800	-0.58263300	1.97696200
H	3.24114200	0.22892800	3.23503300
H	6.18509100	-1.25186900	0.46139600
H	5.37982000	-0.98318800	2.80536800
O	1.38222000	-0.02892100	-1.50251700
H	0.50065100	0.30060600	-1.18110800
N	0.49868900	-2.89676500	0.32573300
C	-0.04571000	-4.12652900	0.98863200

C	-0.19073100	-2.71268800	-1.00953800
C	0.24326000	-1.70653000	1.22227700
C	1.97986500	-3.02056000	0.09885100
H	0.15523200	-4.99319600	0.35468200
H	0.44183400	-4.25262200	1.95791800
H	0.25617400	-1.85606700	-1.50884000
H	-1.25075000	-2.54314500	-0.82826400
H	0.62011400	-0.81649000	0.73136400
H	-0.82965100	-1.62004800	1.38125800
H	2.16735500	-3.88738300	-0.53928100
H	2.47912900	-3.14317400	1.06210400
H	-1.12164800	-3.99468400	1.11957700
H	-0.03327100	-3.62451400	-1.59159800
H	2.32388300	-2.10531100	-0.38440300
H	0.77392600	-1.87312700	2.16215100

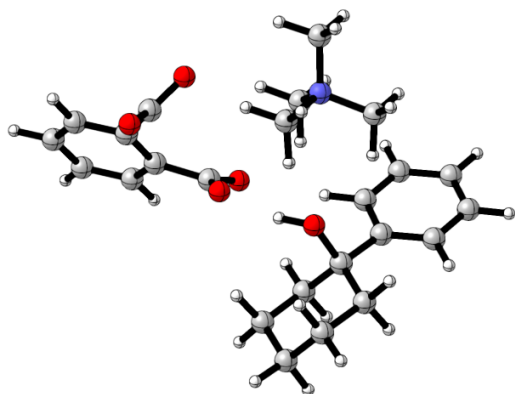
TS+100 (TDRA-1+1e)



C	-5.58468700	1.64921000	1.31770500
C	-4.64221300	2.63586800	1.62827600
C	-3.29456900	2.42018100	1.33536800
C	-2.87860700	1.22566300	0.73311200
C	-3.82080200	0.21265400	0.45081800
C	-5.17345600	0.44974000	0.73477500
C	-3.42445900	-1.17061300	-0.02473700
O	-2.62027600	-1.81625800	0.71291900
O	-3.94334100	-1.60117600	-1.08041200
C	-1.43261800	1.11715200	0.37497000
O	-0.52320200	1.55783100	1.07061600
O	-1.23033900	0.54374200	-0.81558200
H	-6.63717600	1.81205200	1.53631900
H	-4.95515200	3.56923700	2.08879500
H	-2.54972600	3.17834700	1.55900100
H	-5.89596200	-0.32640400	0.49976300
C	1.94827600	2.46874800	-1.11533500
C	2.42509400	1.00232300	-1.27972400
C	3.10784700	1.06773400	-2.69640800
C	2.24779300	2.05311000	-3.52174000
C	1.36724300	2.82037700	-2.49462100
H	1.22162300	2.56767900	-0.30548500
H	2.81796300	3.09664400	-0.87905600
H	4.12220200	1.45685800	-2.54043300
H	3.18659100	0.07318300	-3.14457200
H	2.89332800	2.73379000	-4.08922400

H	1.62708700	1.52064800	-4.24995700
H	1.35416100	3.90079400	-2.67185900
H	0.33077700	2.47230000	-2.55672600
C	3.31559700	0.47078000	-0.15440800
C	2.93061000	0.71101200	1.17611200
C	4.43480200	-0.34004800	-0.39434800
C	3.66085000	0.17054600	2.23735400
H	2.04274400	1.30307100	1.37986000
C	5.16478100	-0.88455300	0.66721100
H	4.74513900	-0.55231100	-1.41339700
C	4.78047200	-0.63062100	1.98811300
H	3.35140600	0.37398000	3.25978400
H	6.03614500	-1.50178800	0.46163800
H	5.35031700	-1.04902100	2.81405500
O	1.35666000	0.12615000	-1.39490200
H	-0.25207200	0.51338200	-1.02838700
N	0.41835200	-2.91481300	0.29576500
C	-0.34327700	-4.02782600	0.96163900
C	-0.19476700	-2.65112900	-1.06371400
C	0.33407200	-1.67653800	1.16039800
C	1.86177500	-3.28365400	0.12390700
H	-0.25284700	-4.92915000	0.35067500
H	0.08543800	-4.20196000	1.95131600
H	0.37626200	-1.85842600	-1.54376500
H	-1.23367100	-2.35645800	-0.91507000
H	0.84576900	-0.86825500	0.64461300
H	-0.71976700	-1.44105800	1.30776400
H	1.93111300	-4.16283900	-0.52056100
H	2.29255400	-3.50158900	1.10346100
H	-1.38679900	-3.71422700	1.03846600
H	-0.13455800	-3.57717900	-1.64084400
H	2.38367900	-2.43751900	-0.32670800
H	0.83437800	-1.89282000	2.10711400

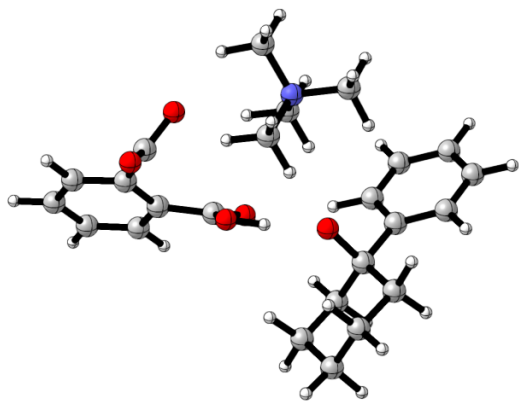
TS-96 (TDRA-1+1b)



C	-5.85766800	-0.95448700	-1.10891900
C	-4.97810100	-1.65485600	-1.95275500
C	-3.59717500	-1.48697600	-1.83261700
C	-3.06286500	-0.63765500	-0.85976300
C	-3.95258500	0.08857200	-0.02902400
C	-5.34738600	-0.08592200	-0.15243300
C	-3.47417600	1.11207900	0.94180900
O	-2.90155900	2.16837100	0.60647200

O	-3.76587400	0.88818800	2.16152800
C	-1.55706600	-0.55194200	-0.68724400
O	-0.85271100	-0.58204000	-1.72312800
O	-1.14475400	-0.46350500	0.50876900
H	-6.93151000	-1.08626300	-1.20852700
H	-5.37597300	-2.33406100	-2.70259300
H	-2.90890600	-2.01571300	-2.48497200
H	-6.01089400	0.47842100	0.49649400
C	3.20682800	-0.47696700	-0.62956900
C	2.49884000	-0.00247800	-1.74998000
C	4.55560600	-0.11505800	-0.50429800
C	3.11699100	0.81043700	-2.70118600
H	1.44973800	-0.25852600	-1.87328000
C	5.17883500	0.70340800	-1.45627600
H	5.14177700	-0.46434400	0.33924600
C	4.46235100	1.17285600	-2.55848900
H	2.54603400	1.15658900	-3.56023200
H	6.22705700	0.96686300	-1.33324600
H	4.94557600	1.80302200	-3.30153900
O	1.49208400	-0.40312700	1.03476300
H	0.56094400	-0.58786500	0.73837800
N	0.58414200	2.92575800	0.77659000
C	0.11835300	4.35049700	0.79380800
C	0.02407500	2.21173400	1.98876800
C	0.09846500	2.26830100	-0.49520300
C	2.08672900	2.85511000	0.81411100
H	0.48089200	4.83461800	1.70344500
H	0.51404900	4.86464800	-0.08487100
H	0.41539500	1.19746500	2.00011100
H	-1.06202100	2.20188800	1.91057100
H	0.43668100	1.23856400	-0.50143400
H	-0.98949700	2.30231800	-0.50823000
H	2.43816700	3.34241900	1.72669400
H	2.48762500	3.36285100	-0.06561700
H	-0.97327900	4.35425300	0.77406100
H	0.35008500	2.76076700	2.87600700
H	2.37137400	1.80200500	0.80337000
H	0.52626000	2.81244300	-1.34009300
C	2.45063500	-1.29610500	0.43243800
C	1.74008100	-2.50837800	-0.21808400
C	3.35540100	-1.78859100	1.57954800
C	0.98291300	-3.37540400	0.80106800
H	2.50842700	-3.11221800	-0.72141000
H	1.04751800	-2.15790500	-0.98977300
C	2.58107900	-2.63031600	2.60465900
H	4.17529200	-2.38889400	1.16061000
H	3.80445400	-0.92073100	2.07896600
C	1.90122900	-3.83618700	1.94102000
H	0.54786500	-4.23987100	0.28156300
H	0.14153300	-2.80322400	1.21298300
H	3.26555400	-2.96161000	3.39715100
H	1.81889300	-1.99773900	3.07708600
H	1.33191700	-4.41036000	2.68411600
H	2.67232000	-4.51275600	1.53881600

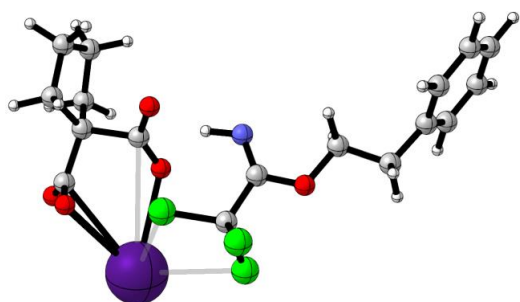
TS+100 (TDRA-1+1b)



C	-5.86830900	-0.77897200	-1.06701300
C	-5.07407700	-1.53795700	-1.93399200
C	-3.68459200	-1.45996300	-1.83857400
C	-3.08068700	-0.62977300	-0.88319500
C	-3.87717700	0.16695600	-0.03279000
C	-5.27147100	0.06371200	-0.12735400
C	-3.29577100	1.22719700	0.88970900
O	-2.66278400	2.16622200	0.31549800
O	-3.50359900	1.11968800	2.11912600
C	-1.59314900	-0.67494700	-0.79751000
O	-0.85387600	-0.86781800	-1.75840800
O	-1.12795500	-0.53857000	0.45107100
H	-6.95243300	-0.83896100	-1.12780700
H	-5.53313200	-2.19217000	-2.67056100
H	-3.04815800	-2.05020800	-2.49158500
H	-5.88289300	0.66436800	0.54023800
C	3.20991600	-0.52333700	-0.65734000
C	2.49206800	-0.14795300	-1.81159100
C	4.51373200	-0.02956600	-0.48055400
C	3.08399600	0.66422400	-2.77976100
H	1.46758700	-0.48174300	-1.94678100
C	5.10410600	0.77841500	-1.45496600
H	5.08741100	-0.29112600	0.40126500
C	4.39160600	1.13094300	-2.60720900
H	2.51876900	0.93363400	-3.66837200
H	6.12411400	1.12825200	-1.31599900
H	4.85288500	1.76182300	-3.36283200
O	1.55562700	-0.47375000	0.86333500
H	-0.13514800	-0.59186300	0.45198500
N	0.42205900	2.97680600	0.93482600
C	-0.40568800	4.23452300	0.96063700
C	-0.02908000	2.07776800	2.06792200
C	0.22696600	2.29084800	-0.39887800
C	1.87723100	3.29218200	1.10562600
H	-0.24540600	4.73778300	1.91703900
H	-0.08630600	4.87987100	0.13891000
H	0.57585500	1.17310800	2.04594900
H	-1.08621900	1.85065200	1.93248900
H	0.82724300	1.38459500	-0.40391400
H	-0.83612100	2.06945900	-0.50674100
H	2.02619400	3.78498000	2.06878500
H	2.19623500	3.95258300	0.29595200
H	-1.45146500	3.93685900	0.84464000

H	0.12694400	2.62158000	3.00298600
H	2.44096400	2.35714100	1.06810800
H	0.57246400	2.97266900	-1.17997700
C	2.49882200	-1.39833000	0.40515200
C	1.83418900	-2.64970500	-0.21573200
C	3.41299200	-1.80995800	1.58289000
C	1.07018100	-3.46643100	0.83903600
H	2.62199900	-3.26660700	-0.67112500
H	1.15009400	-2.34626500	-1.01284900
C	2.63240900	-2.62072400	2.63050200
H	4.24774000	-2.40924400	1.19223900
H	3.83020400	-0.91040300	2.04902900
C	1.97654500	-3.86272900	2.01161000
H	0.63685100	-4.35612900	0.36535900
H	0.22633800	-2.87158000	1.21506700
H	3.30793200	-2.90589500	3.44725400
H	1.85505800	-1.97820700	3.06765600
H	1.40332300	-4.40813500	2.77205100
H	2.76140400	-4.54696100	1.65268400

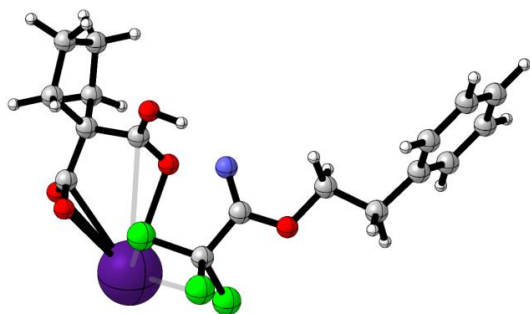
TS-70 (TDRA-4+3a)



C	1.76186300	0.36791000	-1.04708000
O	3.04465000	0.68810100	-0.78983600
C	3.96153900	-0.42709100	-0.72000000
C	5.35401500	0.12949900	-0.43836600
C	0.91722000	1.67130000	-1.05195400
Cl	0.99212000	2.40792200	0.62860700
Cl	-0.79244300	1.36249000	-1.46095700
Cl	1.60669800	2.84679200	-2.22802900
C	6.34752300	-1.00969100	-0.33930500
C	6.63107200	-1.60876900	0.89665000
C	7.49592800	-2.70369900	0.98152000
C	8.09040500	-3.21859200	-0.17453900
C	7.81615000	-2.62943900	-1.41289800
C	6.95143300	-1.53431100	-1.49179200
H	3.62994400	-1.10993100	0.06965900
H	3.92988000	-0.97482000	-1.66749200
H	5.63289500	0.82140100	-1.24206000
H	5.32952000	0.70566500	0.49414900
H	6.17023100	-1.21354300	1.80001100
H	7.70533500	-3.15318700	1.94906800
H	8.76322700	-4.06994100	-0.11099500
H	8.27590600	-3.02096600	-2.31693500
H	6.74182800	-1.08022600	-2.45849600
N	1.37985600	-0.81729100	-1.24077800
O	-4.85545500	-0.66301400	1.07454600

C	-4.16822700	-0.53369300	0.03469300
C	-3.53987400	-1.92911000	-0.42160500
O	-3.88649900	0.47116400	-0.64001000
C	-3.98390300	-2.30070900	-1.83846600
C	-3.81616600	-3.20390000	0.38662700
C	-1.93784100	-1.58894200	-0.21882700
C	-3.66399000	-3.81101500	-1.99587400
H	-5.06762900	-2.12758200	-1.89687800
H	-3.51359300	-1.66101400	-2.58735300
C	-3.36749300	-4.33652100	-0.55903500
H	-3.32493100	-3.20682900	1.36366100
H	-4.89801600	-3.25086100	0.56314600
O	-1.59283300	-1.06327200	0.84564200
O	-1.32379600	-1.98697500	-1.22257800
H	-4.50527200	-4.34281200	-2.45442800
H	-2.79417800	-3.94877600	-2.64461500
H	-2.29358500	-4.51628300	-0.44065600
H	-3.88214200	-5.27790200	-0.33741200
H	0.38082400	-0.96685200	-1.39032100
Cs	-2.56868100	1.56221600	1.97463600

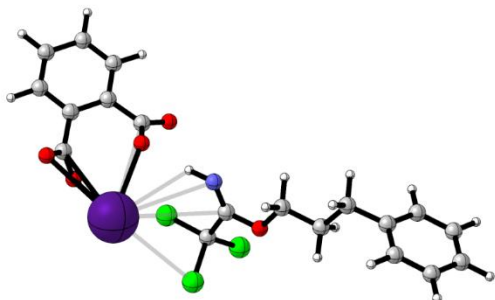
TS+100 (TDRA-4+3a)



C	1.77358500	0.47163200	-1.04604700
O	3.05714100	0.73565300	-0.77600700
C	3.95193000	-0.41181500	-0.72962200
C	5.34932300	0.11443300	-0.42303600
C	0.88951500	1.73308700	-1.04072500
Cl	1.01002900	2.47633400	0.62540300
Cl	-0.80673500	1.32381900	-1.37922200
Cl	1.52983800	2.89677400	-2.25233200
C	6.33315100	-1.03460500	-0.33536500
C	6.60957900	-1.64809900	0.89496200
C	7.47878900	-2.74019300	0.97023200
C	8.08287600	-3.23605700	-0.18909300
C	7.81451000	-2.63210900	-1.42155000
C	6.94580800	-1.53963600	-1.49176500
H	3.59763400	-1.09997900	0.04644000
H	3.91587400	-0.92590500	-1.69689500
H	5.64204800	0.81982400	-1.20976500
H	5.31804000	0.67172700	0.52047300
H	6.14463800	-1.26486800	1.80136000
H	7.68521400	-3.20095000	1.93286600
H	8.76010800	-4.08415700	-0.13241300
H	8.28360300	-3.00821900	-2.32709700
H	6.74530600	-1.07019200	-2.45313900

N	1.29491000	-0.67500300	-1.28864300
O	-4.73584300	-0.40733400	0.98909300
C	-3.98766300	-0.47877000	-0.01821000
C	-3.41889900	-1.87377700	-0.42283600
O	-3.55560300	0.49844900	-0.70264600
C	-3.87806600	-2.30606800	-1.83512600
C	-3.89261600	-3.05578800	0.45391000
C	-1.91017700	-1.72076000	-0.27395500
C	-3.74446600	-3.85202100	-1.87481300
H	-4.92924400	-2.01250100	-1.93964100
H	-3.32025400	-1.79807500	-2.62407900
C	-3.57893300	-4.30552600	-0.39288700
H	-3.42263200	-3.06045300	1.44244700
H	-4.97000500	-2.93182400	0.60872300
O	-1.37453600	-1.25529200	0.72890600
O	-1.19029400	-2.13692000	-1.32685400
H	-4.62735200	-4.30763900	-2.33813700
H	-2.87694900	-4.15337700	-2.47089700
H	-2.54558400	-4.62966000	-0.21325200
H	-4.22633200	-5.15184600	-0.13439300
H	-0.25286900	-1.87443200	-1.18979400
Cs	-2.62537900	1.51923700	1.97995200

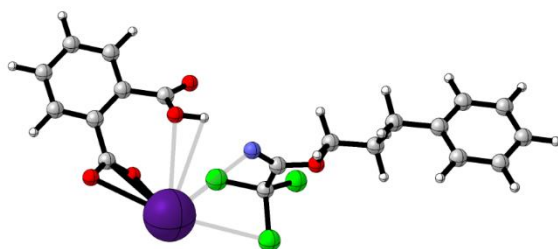
TS-70 (TDRA-3+3b)



C	4.74963300	-0.68034900	0.35132600
C	5.52034100	-1.86958000	-0.25667900
C	3.25944100	-0.84202400	0.12414000
O	2.58692600	0.28798400	0.72273100
C	1.24336300	0.21303100	0.73516600
C	0.67644900	1.48013700	1.43580100
N	0.61303400	-0.73988900	0.20145900
H	-0.40815900	-0.76606300	0.29700900
C	-4.68025300	0.09344000	-0.76524400
O	-4.23921600	1.04653300	-0.06672000
O	-4.76542000	0.16288700	-2.02159000
C	-2.75934200	-1.58111000	0.76315400
O	-2.19319200	-1.14232000	-0.27678700
O	-2.18000900	-1.76973600	1.86330300
Cl	1.47153500	1.75875800	3.01738000
Cl	1.03388200	2.89830100	0.31548900
Cl	-1.08779800	1.38591600	1.66891600
C	7.00939400	-1.74710300	-0.03072300
C	7.60245100	-2.26717500	1.12862300
C	8.96791300	-2.09765800	1.37275600
C	9.76314400	-1.40316200	0.45570700
C	9.18388500	-0.88457200	-0.70667700

C	7.81788900	-1.05739200	-0.94538200
C	-5.12666000	-1.15731900	-0.07797400
C	-6.46834300	-1.56044500	-0.18330100
C	-6.91126800	-2.69429300	0.48802300
C	-6.01817900	-3.44592600	1.27714300
C	-4.68722300	-3.05918000	1.38613600
C	-4.22218600	-1.92390100	0.70377500
H	4.95248700	-0.61716300	1.42742900
H	5.09901000	0.25875500	-0.09557000
H	5.30935700	-1.92717600	-1.33331900
H	5.15109700	-2.80439400	0.18612100
H	2.87383800	-1.76040400	0.57984200
H	3.00744900	-0.87473800	-0.94313100
H	6.98840800	-2.80851700	1.84605200
H	9.41065200	-2.50916900	2.27649500
H	10.82563500	-1.27096500	0.64318100
H	9.79551800	-0.34822300	-1.42811200
H	7.37243800	-0.65200000	-1.85221700
H	-7.15042800	-0.97045000	-0.78862400
H	-7.95008100	-3.00258400	0.40452500
H	-6.37053600	-4.33353100	1.79588600
H	-3.98362400	-3.62630100	1.98736200
Cs	-1.72963000	1.26194400	-2.05689800

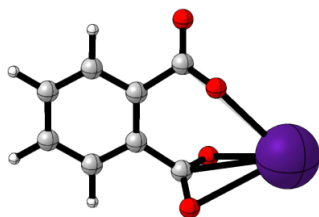
TS+100 (TDRA-3+3b)



C	4.73303800	-0.74903800	0.43633500
C	5.51166000	-1.88579000	-0.25729700
C	3.24580100	-0.85391300	0.16048600
O	2.59244200	0.24544600	0.86162700
C	1.27305900	0.33694100	0.71313200
C	0.64989700	1.55046700	1.43752300
N	0.55738900	-0.42415100	-0.00742500
H	-1.12373300	-1.46689300	0.01641100
C	-4.39427700	0.07702400	-0.70500800
O	-3.71668000	0.83835600	0.04890700
O	-4.60381400	0.24155700	-1.93936500
C	-2.73096400	-1.82508500	0.95329200
O	-2.06913000	-1.59112500	-0.21237400
O	-2.13245900	-1.96628300	2.00502600
Cl	1.38393400	1.77416200	3.04861600
Cl	1.03653500	2.99316900	0.37657600
Cl	-1.11190500	1.35270900	1.55352900
C	7.00265900	-1.75922400	-0.03074000
C	7.59855200	-2.29258700	1.12124900
C	8.96527400	-2.12791200	1.36178900
C	9.75848600	-1.42570100	0.44874600
C	9.17613100	-0.89327500	-0.70544800
C	7.80845300	-1.06041200	-0.94077900

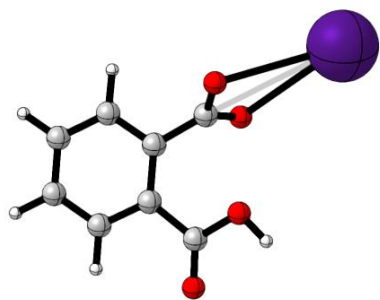
C	-4.97533800	-1.16737200	-0.05616400
C	-6.33161600	-1.46612800	-0.22768300
C	-6.92182800	-2.53722000	0.44759500
C	-6.15568400	-3.33437700	1.30521300
C	-4.79714800	-3.06173900	1.46774700
C	-4.20131900	-1.99436100	0.78049900
H	4.90675100	-0.78467600	1.51840800
H	5.10030900	0.22231300	0.08355400
H	5.29789100	-1.87015100	-1.33467400
H	5.15564600	-2.85348500	0.12091700
H	2.81904400	-1.79433600	0.52887000
H	3.02099100	-0.76280200	-0.90940700
H	6.98771700	-2.84312500	1.83448100
H	9.41069800	-2.55071900	2.25876700
H	10.82205000	-1.29886600	0.63302700
H	9.78601400	-0.35147600	-1.42401800
H	7.36212400	-0.64575300	-1.84295300
H	-6.91701600	-0.83814400	-0.89304800
H	-7.98014300	-2.74679000	0.30981700
H	-6.61101000	-4.16533000	1.83791800
H	-4.18122600	-3.67569000	2.11881000
Cs	-1.81721500	1.30856100	-2.13410500

Asynchronicity Factor TDRA-3⁻



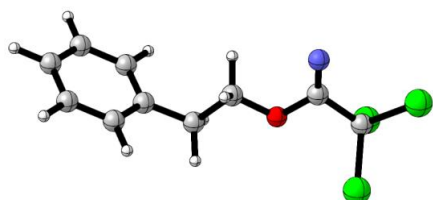
C	-4.06884400	-1.23567000	0.20270500
C	-4.35037800	0.13310000	0.27965600
C	-3.30649100	1.05540900	0.17125900
C	-1.97292800	0.65035200	-0.00365000
C	-1.69503000	-0.73294200	-0.09633200
C	-2.74893400	-1.65373300	0.01613400
C	-0.30637800	-1.29793700	-0.36474100
O	0.22046900	-1.01873400	-1.48124300
O	0.22211600	-2.00132100	0.54884900
C	-0.90343100	1.75948600	-0.02230500
O	0.19766700	1.48630700	0.55712600
O	-1.22353800	2.84545700	-0.55883300
H	-4.86876500	-1.97093700	0.28570900
H	-5.37370000	0.47900600	0.42270200
H	-3.50293500	2.12351500	0.21304300
H	-2.51539100	-2.71511600	-0.04008800
Cs	2.49166500	-0.00870100	0.09991100

TDRA-3H⁺



H	0.88691900	2.98437200	0.48113100
C	0.43553400	-0.55955200	-0.01457100
O	-0.25937100	-0.89976500	0.98298200
O	-0.18656000	-0.21742100	-1.05423800
C	2.35012800	1.87295900	0.05340600
O	1.06222100	2.02409600	0.45411100
O	3.07256600	2.81098100	-0.19878000
C	1.91109500	-0.66963100	0.01866100
C	2.43294000	-1.98315200	0.02108400
C	3.80757100	-2.19299200	-0.01753100
C	4.67405600	-1.09380600	-0.06506100
C	4.16448300	0.21387900	-0.05902000
C	2.79072500	0.44359900	-0.00442400
H	1.74817200	-2.82546500	0.04408800
H	4.20354600	-3.20377400	-0.01601900
H	5.74825700	-1.24860500	-0.10205000
H	4.83292400	1.06825200	-0.08702800
Cs	-3.31508900	-0.04919500	-0.02523600

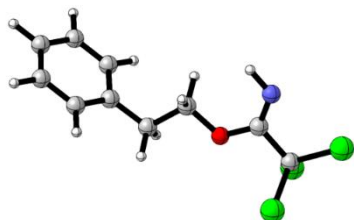
3a⁻



C	-1.49182400	-0.08217000	0.75262600
O	-0.49341100	0.04064000	-0.13072200
C	0.87331800	-0.01258800	0.36336000
C	1.79675700	0.11474900	-0.84515700
C	-2.84105900	-0.00145300	0.00186400
Cl	-2.94391400	1.58622000	-0.85690000
Cl	-4.23406300	-0.14822800	1.10881900
Cl	-2.91870900	-1.33858700	-1.21307100
C	3.25235900	0.05420700	-0.42600700
C	3.96065400	1.22657200	-0.11716100
C	5.29710200	1.16917900	0.29285900
C	5.94609800	-0.06577200	0.40152300
C	5.25028100	-1.24094400	0.09574000
C	3.91440900	-1.17926300	-0.31446900
H	1.02217800	0.81086100	1.07036100
H	1.02320800	-0.96698800	0.87970700
H	1.57322600	-0.69736000	-1.54528300
H	1.58924700	1.06376000	-1.35086600
H	3.46368500	2.19010600	-0.20500400
H	5.83084000	2.08764700	0.52310000

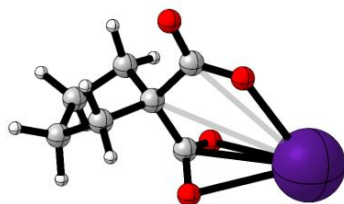
H	6.98495000	-0.11187900	0.71714600
H	5.74738500	-2.20449800	0.17240300
H	3.38124900	-2.09601400	-0.55644900
N	-1.46563000	-0.24357000	2.00991000
H	-0.51418400	-0.28075400	2.37981900

3aH⁺



C	-1.51077800	-0.30184800	0.66803400
O	-0.46962000	0.07080200	-0.09784300
C	0.85483300	-0.14318000	0.41772400
C	1.79497500	0.45747800	-0.64392100
C	-2.84217100	0.01224000	-0.03688000
Cl	-2.94049800	1.78374800	-0.32127600
Cl	-4.20075300	-0.50906700	0.99891800
Cl	-2.89479800	-0.87646000	-1.59772300
C	3.23878200	0.22190000	-0.33271500
C	4.06720000	1.28021100	0.14391900
C	5.39154200	1.04401500	0.45162400
C	5.93266800	-0.25962300	0.28215400
C	5.12584300	-1.32204900	-0.19899700
C	3.80239100	-1.08423600	-0.50430000
H	0.97119900	0.36929700	1.38081800
H	1.02966100	-1.21781600	0.55129900
H	1.54122600	-0.02122000	-1.60100600
H	1.57851700	1.52600700	-0.73305900
H	3.64227000	2.27290400	0.26214400
H	6.02586400	1.84483000	0.81880300
H	6.97748400	-0.44141500	0.51815200
H	5.55690100	-2.30954600	-0.33045200
H	3.17408100	-1.88352600	-0.88832900
N	-1.51777200	-0.83659400	1.81305900
H	-0.63471200	-1.04898200	2.27449400

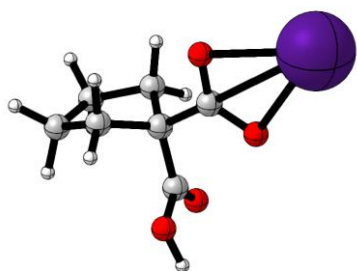
TDRA-4⁻



C	-3.56815000	-1.04806300	-0.78095700
C	-2.61687200	0.10089500	-1.19298100
C	-1.64926800	0.25885800	-0.00001900
C	-2.61678400	0.10082300	1.19297200
C	-3.56792800	-1.04824600	0.78097100
H	-4.57787100	-0.91592900	-1.19661000
H	-3.18583200	-2.00415500	-1.16067900

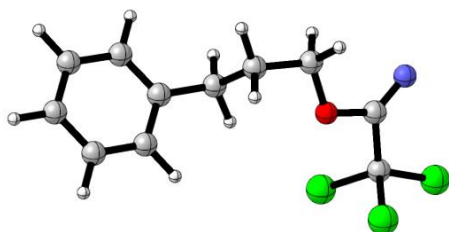
H	-3.16975200	1.04179400	-1.30240300
H	-2.07826100	-0.10791900	-2.12183800
H	-2.07813700	-0.10790900	2.12182500
H	-3.16978600	1.04165800	1.30238700
H	-3.18519000	-2.00431300	1.16033200
H	-4.57754900	-0.91647600	1.19696600
C	-0.96992100	1.69300400	0.00006000
C	-0.56105400	-0.85442400	-0.00006200
O	0.30482300	1.74089000	0.00018600
O	-0.10626800	-1.24086700	-1.12270600
O	-1.75163800	2.67080100	0.00001200
O	-0.10649800	-1.24121000	1.12256500
Cs	2.41088900	-0.12146800	-0.00000600

TDRA-4H⁺



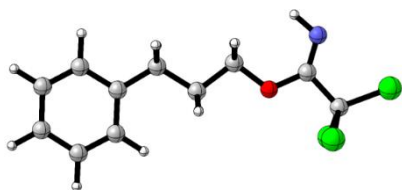
O	-0.30275900	-1.16657400	0.21367200
C	0.28651800	-0.07331700	-0.01375900
C	1.84234200	-0.10091800	-0.00729000
O	-0.28639000	1.03239000	-0.26391000
C	2.39277200	-0.95065900	-1.17681500
C	2.43143800	-0.84035800	1.21677500
C	2.34440000	1.33569600	-0.10164600
C	3.82861400	-1.35237600	-0.75000800
H	1.75371100	-1.83553400	-1.26450500
H	2.36583800	-0.40322800	-2.12258200
C	3.87941400	-1.16826600	0.79741800
H	2.37100600	-0.25446000	2.13874500
H	1.84273400	-1.75431900	1.35008800
O	2.27573100	1.98812400	1.08622800
O	2.75856300	1.87674600	-1.10910900
H	4.05321500	-2.38391700	-1.04580200
H	4.56869500	-0.70977800	-1.23925100
H	4.54059200	-0.33203700	1.05785200
H	4.26579800	-2.05332800	1.31640900
Cs	-3.01440100	-0.07570500	-0.00548900
H	2.43633600	2.94609100	0.90783500

3b⁻



C	1.40891500	1.48540200	-0.78050700
C	1.88154900	0.70739600	0.46613400
C	-0.02716300	1.98273000	-0.63819700
O	-0.85363400	0.84699100	-0.49069400
C	-2.22102300	1.16242400	-0.13316300
C	-2.85366200	-0.25414600	0.07515500
N	-2.77416100	2.24667600	-0.00342600
Cl	-1.97710100	-1.21455800	1.41813800
Cl	-4.58287500	-0.14418300	0.54440900
Cl	-2.76479100	-1.30129300	-1.46493100
C	3.26644600	0.12932500	0.29704500
C	3.45051400	-1.10435000	-0.34993800
C	4.72920500	-1.63027400	-0.55275100
C	5.85755100	-0.93047500	-0.10956900
C	5.69089200	0.29839200	0.53701500
C	4.40780500	0.81896300	0.73548000
H	2.07739900	2.34152900	-0.95944900
H	1.47899000	0.83155900	-1.66059400
H	1.15403500	-0.08788000	0.66119300
H	1.85825700	1.37974400	1.33489300
H	-0.32956200	2.56930200	-1.51991800
H	-0.13585000	2.64687000	0.23337500
H	2.57586200	-1.65298000	-0.69360500
H	4.84514200	-2.58938300	-1.05339800
H	6.85362700	-1.33978600	-0.26360600
H	6.55944100	0.85120900	0.88972900
H	4.28572000	1.77540900	1.24120900

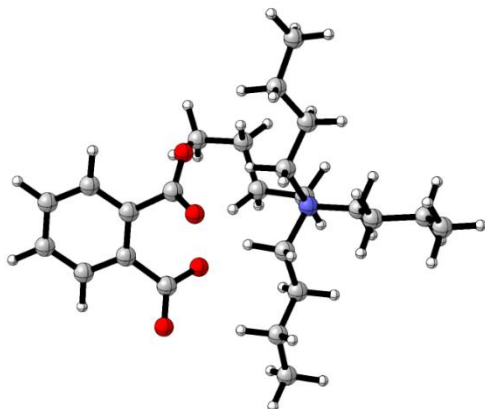
3bH⁺



C	1.35469900	0.31476500	0.00009800
C	2.65553300	1.11991700	0.00005900
C	0.13729300	1.23345800	0.00011100
O	-1.00221600	0.37555000	0.00016500
C	-2.24346700	0.92703300	0.00006000
C	-3.28870600	-0.20801900	-0.00000600
Cl	-3.02581800	-1.21910800	-1.47619500
Cl	-3.02612500	-1.21901900	1.47630100
Cl	-4.94925400	0.40955000	-0.00019500
C	3.93927500	0.35773300	-0.00000400
C	5.17205700	1.10935700	-0.00017000
C	6.39164600	0.47084700	-0.00021900
C	6.43044700	-0.94388400	-0.00010400
C	5.22345800	-1.70517800	0.00006000
C	4.00178600	-1.06626800	0.00010800
H	1.29815400	-0.33077100	-0.88407300
H	1.29818600	-0.33074300	0.88429100
H	2.68594200	1.80619200	0.86695500
H	2.68587000	1.80624400	-0.86679400
H	0.12190100	1.87430400	-0.89351500
H	0.12195400	1.87434600	0.89370700

H	5.11780000	2.19497000	-0.00025500
H	7.31644100	1.03895100	-0.00034500
H	7.38692900	-1.45934400	-0.00014100
H	5.27809000	-2.78956600	0.00014500
H	3.08649800	-1.64713900	0.00023100
N	-2.59680700	2.13964200	0.00000000
H	-1.82614200	2.80790400	0.00004900

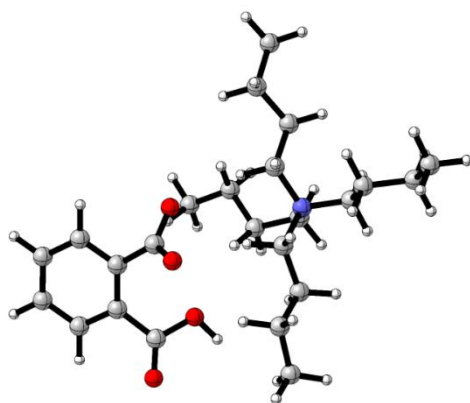
TDRA-1⁻



C	-5.90689300	0.02068100	-0.80423800
C	-5.49435400	-1.26891900	-1.15863800
C	-4.12925600	-1.56774200	-1.19032300
C	-3.16011900	-0.60201900	-0.87804900
C	-3.57566700	0.69259500	-0.49955600
C	-4.94791900	0.98535400	-0.48252200
C	-2.61410000	1.78253400	-0.01747000
O	-2.79300100	2.94639500	-0.45705900
O	-1.74864400	1.41647300	0.83748200
C	-1.69546500	-0.99813100	-1.03910400
O	-1.32479900	-2.06003600	-0.44153100
O	-0.97817800	-0.26773500	-1.77234200
H	-6.96662900	0.27251500	-0.77676900
H	-6.22807400	-2.03423500	-1.40986200
H	-3.79051300	-2.56650500	-1.45686000
H	-5.24735900	1.99545200	-0.21351100
N	1.92359600	0.11413800	0.56115300
C	1.54667200	-0.13459100	2.02613300
C	1.60422900	-1.10059300	-0.30385700
C	1.10957700	1.28236700	-0.02671900
C	3.40525300	0.42566400	0.55462400
H	2.24492000	-0.89885900	2.38379100
H	1.79964900	0.79864500	2.53325700
C	0.09676900	-0.53727500	2.32140300
H	1.69864800	-0.77420200	-1.34047700
H	0.53944100	-1.31553900	-0.18020100
C	2.42962400	-2.35558300	-0.04181800
H	1.49672200	1.42242700	-1.03739000
H	0.08116600	0.93641300	-0.13030800
C	1.12809200	2.57851400	0.77220900
H	3.90416000	-0.43256100	1.01300900
H	3.55035000	1.27908200	1.22145300
C	4.03019700	0.72194100	-0.80749500
H	-0.60070000	-0.10522700	1.59407700
H	-0.16527700	-0.04575800	3.26960800

C	-0.14774200	-2.04562500	2.47399300
H	2.38500400	-2.63852700	1.01784000
H	3.49268800	-2.21706300	-0.29274100
C	1.85428700	-3.50737100	-0.88559100
H	2.14553400	2.87323600	1.07858300
H	0.51301600	2.45178100	1.66951000
C	0.50219300	3.70380900	-0.06785800
H	3.81689000	-0.08863300	-1.51359900
H	3.60206100	1.63628700	-1.23265600
C	5.55153400	0.89228000	-0.67667900
H	0.07214700	-2.56269600	1.53622300
H	0.52368900	-2.45342200	3.25048100
C	-1.61146100	-2.33174600	2.82497100
H	1.95113500	-3.25350400	-1.95066000
H	0.77645100	-3.57977500	-0.69589100
C	2.55221200	-4.84163000	-0.60291400
H	1.10511000	3.86244500	-0.97663100
H	-0.50429700	3.39702500	-0.37661000
C	0.39402500	5.01203400	0.72104900
H	5.98863400	-0.02749100	-0.26108500
H	5.77004900	1.69270700	0.04529800
C	6.21957800	1.21630400	-2.01822000
H	-2.24931200	-2.00463400	1.99790700
H	-1.91591000	-1.80432700	3.74040800
H	-1.77788800	-3.40629800	2.97780100
H	2.13795400	-5.64531500	-1.22420700
H	2.42640200	-5.13586600	0.44786300
H	3.63164600	-4.78398900	-0.80516700
H	1.37485000	5.35921100	1.08239200
H	-0.26321700	4.87531300	1.58866000
H	-0.04163600	5.80623400	0.10256000
H	6.03943000	0.41834000	-2.74976900
H	7.30454700	1.33225600	-1.90655700
H	5.82271600	2.14819200	-2.44024000

TDRA-1H⁺

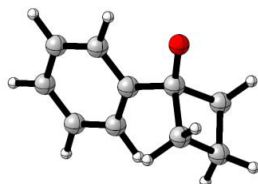


C	-6.21807200	-0.96207500	-0.52033500
C	-5.47026700	-1.98925900	-1.10458400
C	-4.09760200	-1.82773200	-1.28913300
C	-3.46422900	-0.64291800	-0.87605500
C	-4.21442600	0.38572200	-0.25843500
C	-5.59244200	0.21742900	-0.10195900

C	-3.62632200	1.64170400	0.29819600
O	-4.22842100	2.68589100	0.41021600
C	-2.03217900	-0.51169800	-1.20776400
O	-1.18163100	-1.40455600	-0.93549600
O	-1.55125500	0.46799000	-1.84598200
H	-7.28948800	-1.07722200	-0.38583500
H	-5.95579000	-2.90522000	-1.42728400
H	-3.50945700	-2.60305500	-1.77074600
H	-6.16464900	1.01386400	0.36282600
N	2.22912400	0.16904400	0.47844300
C	1.70017700	-0.08402700	1.89470100
C	2.18267900	-1.09929300	-0.37406900
C	1.36691200	1.20164200	-0.25336100
C	3.66389300	0.67394400	0.64161500
H	2.38130000	-0.80823400	2.34611700
H	1.85041000	0.86205200	2.41702300
C	0.24367300	-0.55097800	2.03307100
H	2.47003300	-0.79178100	-1.38227900
H	1.13270500	-1.38575500	-0.41914500
C	3.04890200	-2.26375400	0.09515100
H	1.88812500	1.41780900	-1.18732600
H	0.44275000	0.69318200	-0.52152800
C	1.05228300	2.49246800	0.49625900
H	4.17205200	-0.06480200	1.26538900
H	3.59529100	1.59584700	1.22312600
C	4.46068600	0.91681400	-0.63849600
H	-0.39467100	-0.09992900	1.26877500
H	-0.11016800	-0.13306200	2.98518800
C	0.01564100	-2.07143500	2.07308500
H	2.80342300	-2.54389900	1.12579200
H	4.11258700	-1.99695100	0.07636900
C	2.82230900	-3.48407200	-0.81546100
H	1.96348100	2.99396200	0.84519900
H	0.44711700	2.27583300	1.38508300
C	0.27025400	3.44817200	-0.42504400
H	4.54026600	-0.00227100	-1.23044200
H	3.97117400	1.66687300	-1.27057900
C	5.87814000	1.40916400	-0.29202800
H	0.29825000	-2.53352300	1.12135800
H	0.66279500	-2.51334800	2.84387900
C	-1.44916600	-2.40984900	2.37218700
H	3.05401000	-3.21219300	-1.85462800
H	1.75819300	-3.75656600	-0.79615000
C	3.67322600	-4.68662000	-0.39295100
H	0.91150700	3.74643200	-1.26520100
H	-0.58027000	2.91215000	-0.86562200
C	-0.21992500	4.69750200	0.31535300
H	6.37798900	0.66377400	0.34209800
H	5.80981700	2.32982800	0.30396800
C	6.72141500	1.66781600	-1.54565100
H	-2.10841700	-2.00129400	1.59770800
H	-1.76404700	-1.99542300	3.33790700
H	-1.60333100	-3.49365300	2.40658900
H	3.49572200	-5.54270700	-1.05226900
H	3.43657100	-4.99880100	0.63172300
H	4.74362000	-4.45005000	-0.43356700
H	0.61714900	5.26607000	0.73813900

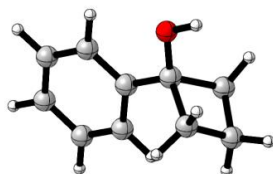
H	-0.89134800	4.44033800	1.14668200
H	-0.77256900	5.36119300	-0.35710200
H	6.83342300	0.75510200	-2.14363100
H	7.72410100	2.01587900	-1.27674800
H	6.26129300	2.43317600	-2.18255200
O	-2.34437300	1.48932400	0.73239300
H	-2.06274700	2.36188700	1.06779400

1a⁻



C	3.08015300	-0.40269900	0.00009300
C	2.13226900	-1.43381900	-0.00010400
C	0.76475900	-1.13373900	-0.00020400
C	0.30337200	0.19470400	-0.00010800
C	1.26698700	1.21457800	0.00006800
C	2.63551200	0.92564900	0.00017500
C	-1.19671100	0.61558200	-0.00014600
H	4.14514200	-0.63213100	0.00017200
H	2.45880500	-2.47411500	-0.00019000
H	0.05056000	-1.95481600	-0.00037700
H	3.36158900	1.73927600	0.00031300
C	-2.00943900	-0.24873800	-1.10191900
C	-2.57652300	-1.17922000	0.00037700
C	-2.00928800	-0.24815400	1.10208800
H	-3.66734400	-1.31984600	0.00049200
H	-2.11978000	-2.17890400	0.00062500
H	-1.42870700	-0.72722600	1.90491200
H	-2.76356400	0.41324600	1.54090900
H	-1.42895800	-0.72823800	-1.90454900
H	-2.76377000	0.41246200	-1.54094000
O	-1.38394300	1.92422500	-0.00042200
H	0.88103400	2.23163000	0.00009300

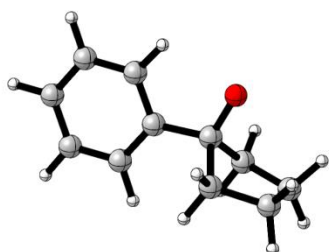
1aH⁺



C	3.06877700	-0.43746600	0.00051800
C	2.10727300	-1.47515700	-0.00180000
C	0.76482900	-1.16197700	-0.00247900
C	0.33679400	0.20569500	-0.00127400
C	1.32207800	1.24027500	0.00143700
C	2.66443300	0.91980000	0.00211200
C	-1.09644600	0.53075700	-0.00210100
H	4.12682800	-0.68419700	0.00120400
H	2.42989200	-2.51145800	-0.00299300

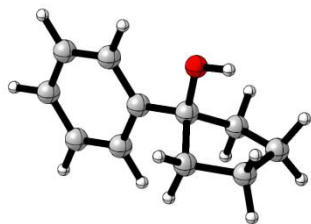
H	0.02991200	-1.95995600	-0.00412500
H	3.41436100	1.70468600	0.00387000
C	-1.98623800	-0.30903200	-1.08572900
C	-2.61342400	-1.19645100	0.00355100
C	-1.98323800	-0.30632300	1.08853700
H	-3.70421400	-1.23800900	0.00522800
H	-2.23459400	-2.22158000	0.00442300
H	-1.38134700	-0.78247600	1.86413700
H	-2.67367900	0.40870300	1.54407100
H	-1.38703700	-0.78774300	-1.86189100
H	-2.67880800	0.40365100	-1.54173000
O	-1.27829400	1.90002000	-0.00337400
H	-2.22081800	2.13379300	-0.00446600
H	0.99682900	2.27370400	0.00264000

1e⁻



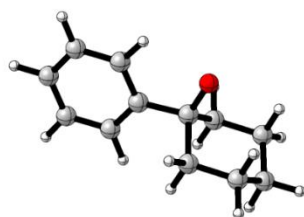
C	1.54903500	0.34269300	-1.19823700
C	0.84043000	-0.40339600	-0.00000500
C	1.54909200	0.34270300	1.19823900
C	3.03599900	0.34366000	0.78203100
C	3.03598000	0.34402000	-0.78205300
H	1.35992400	-0.20482500	-2.12867900
H	1.18650100	1.37655100	-1.32515100
H	1.18674600	1.37663900	1.32506000
H	1.35985700	-0.20473700	2.12870000
H	3.58139300	1.20570100	1.19526400
H	3.52321800	-0.56438600	1.15217200
H	3.58096300	1.20651400	-1.19487900
H	3.52363700	-0.56360300	-1.15265900
C	-0.68512800	-0.10063100	0.00001700
C	-1.56882600	-1.19029100	-0.00005600
C	-1.24358900	1.19028300	0.00006300
C	-2.95536100	-1.00368200	-0.00006600
H	-1.10514500	-2.17438900	-0.00007900
C	-2.62940000	1.38789100	0.00007100
H	-0.58850000	2.05974600	0.00009500
C	-3.49711000	0.28794300	0.00000600
H	-3.61947800	-1.86854500	-0.00012900
H	-3.03355000	2.40048600	0.00012600
H	-4.57626500	0.43731200	0.00001000
O	1.12924600	-1.71620200	0.00001100

1eH⁺



C	1.51518600	-0.36493900	1.21630000
C	0.77489000	0.33936400	-0.00007500
C	1.51541900	-0.36523000	-1.21623500
C	2.99827400	-0.38632900	-0.77659800
C	2.99815800	-0.38636500	0.77681500
H	1.31795700	0.19574400	2.13382400
H	1.12971900	-1.37956100	1.34352900
H	1.13005400	-1.37993700	-1.34313700
H	1.31819400	0.19514600	-2.13394900
H	3.49451200	-1.26814000	-1.19375600
H	3.53150000	0.48373000	-1.17505500
H	3.49400000	-1.26841300	1.19392800
H	3.53159400	0.48350100	1.17538300
C	-0.68825200	0.11872100	-0.00002300
C	-1.21906100	-1.21837600	-0.00003600
C	-1.59847500	1.22328200	0.00001900
C	-2.57903200	-1.43352900	-0.00004400
H	-0.54275400	-2.06627600	-0.00007400
C	-2.95822300	1.00158900	0.00006900
H	-1.19616900	2.22895300	-0.00011800
C	-3.46211500	-0.32683500	0.00002500
H	-2.97721100	-2.44316300	-0.00008500
H	-3.65090600	1.83750300	0.00010500
H	-4.53566200	-0.49440500	-0.00006800
O	1.02456000	1.72076100	-0.00022300
H	1.97807700	1.90111700	-0.00005600

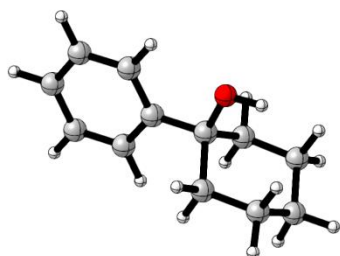
1b



C	-0.97068500	-0.10199400	-0.00011800
C	-1.87705600	-1.17231000	-0.00026900
C	-1.49927200	1.20084400	0.00024300
C	-3.25918300	-0.95518100	-0.00013100
H	-1.43472600	-2.16623800	-0.00046000
C	-2.88066400	1.42887700	0.00039700
H	-0.82508800	2.05549800	0.00034200
C	-3.77202000	0.34828400	0.00016700
H	-3.94244200	-1.80499800	-0.00032000
H	-3.26263600	2.45005100	0.00070800
H	-4.84763700	0.52137100	0.00036400
O	0.80588800	-1.75883800	-0.00097900
C	0.55365200	-0.43733500	-0.00029400

C	1.19012500	0.26541900	-1.26625000
C	1.19007800	0.26405600	1.26654600
C	2.70984300	0.05600500	-1.26920600
H	0.96804500	1.34676600	-1.29708900
H	0.73848200	-0.19282000	-2.15652500
C	2.70981200	0.05466100	1.26935500
H	0.96800100	1.34535800	1.29857300
H	0.73836700	-0.19514500	2.15629000
C	3.35196000	0.64210300	0.00039800
H	3.16664100	0.50408600	-2.16703500
H	2.89214700	-1.02599100	-1.29858900
H	3.16657600	0.50176600	2.16769400
H	2.89209700	-1.02736200	1.29758700
H	4.43890000	0.45933100	0.00027600
H	3.21662600	1.73845600	0.00098300

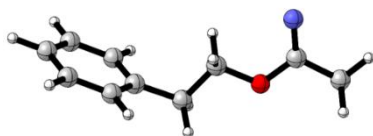
1bH⁺



C	-0.97348300	-0.12470000	0.00648800
C	-1.91781600	-1.19764600	0.00272500
C	-1.45953000	1.22636500	0.00007500
C	-3.27083700	-0.93219900	-0.00224900
H	-1.55016100	-2.21645800	0.00587300
C	-2.81291400	1.48620600	-0.00466600
H	-0.75724700	2.05272200	-0.00003900
C	-3.73160800	0.41030700	-0.00606700
H	-3.98939000	-1.74598900	-0.00315900
H	-3.17701900	2.50864700	-0.00789400
H	-4.79903500	0.61293400	-0.01090700
O	0.68427000	-1.77957700	0.02751900
H	1.63091400	-1.99061400	0.04420000
C	0.48543300	-0.39316700	0.01340300
C	1.16398400	0.24815800	-1.29089200
C	1.17785600	0.28057700	1.28627600
C	2.68301000	0.07525600	-1.26975500
H	0.91164300	1.31165100	-1.33302900
H	0.70929300	-0.24977200	-2.15230400
C	2.69706800	0.10864800	1.25635800
H	0.92721200	1.34518900	1.30379900
H	0.73273900	-0.19228000	2.16692800
C	3.32515800	0.69036800	-0.01839400
H	3.07865500	0.55852800	-2.17320100
H	2.95271600	-0.98672600	-1.35872600
H	3.10283400	0.61528300	2.14197300
H	2.97009300	-0.95033000	1.37054400
H	4.40578300	0.51512600	-0.02212900
H	3.17888900	1.77966400	-0.03189500

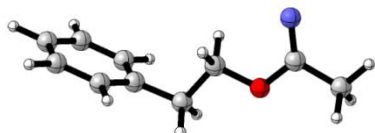
BDFE

S4-



N	-3.27186700	0.00002300	1.63828400
C	-3.38781300	-0.00001700	0.37480800
O	-2.33880300	-0.00003300	-0.49122400
C	-1.01848300	-0.00001100	0.09713500
C	-0.01065700	-0.00002900	-1.05003000
C	1.40917300	-0.00001200	-0.52346700
C	2.07279100	1.20565900	-0.25226700
C	3.36684300	1.20853300	0.27599400
C	4.01799800	0.00002200	0.54229400
C	3.36686100	-1.20850500	0.27602800
C	2.07280900	-1.20566600	-0.25223400
H	-0.90445200	0.88814200	0.73050100
H	-0.90444300	-0.88813800	0.73053700
H	-0.19066000	-0.88267400	-1.67542600
H	-0.19066900	0.88258800	-1.67546100
H	1.57278700	2.14968800	-0.46076000
H	3.86659600	2.15303100	0.47616300
H	5.02524300	0.00003500	0.95081000
H	3.86662800	-2.15299100	0.47622400
H	1.57281900	-2.14970800	-0.46070000
C	-4.71905100	0.00002800	-0.33399700
H	-4.79204000	-0.88801200	-0.97144300
H	-5.53918700	0.00008400	0.38725500
H	-4.79195600	0.88804200	-0.97148800

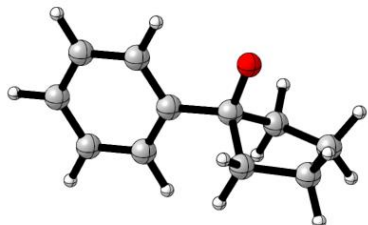
S4-IM



N	3.27186700	-0.00002300	1.63828400
C	3.38781300	0.00001700	0.37480800
O	2.33880300	0.00003300	-0.49122400
C	1.01848300	0.00001100	0.09713500
C	0.01065700	0.00002900	-1.05003000
C	-1.40917300	0.00001200	-0.52346700
C	-2.07279100	-1.20565900	-0.25226700
C	-3.36684300	-1.20853300	0.27599400
C	-4.01799800	-0.00002200	0.54229400
C	-3.36686100	1.20850500	0.27602800
C	-2.07280900	1.20566600	-0.25223400
H	0.90445200	-0.88814200	0.73050100
H	0.90444300	0.88813800	0.73053700
H	0.19066000	0.88267400	-1.67542600
H	0.19066900	-0.88258800	-1.67546100
H	-1.57278700	-2.14968800	-0.46076000
H	-3.86659600	-2.15303100	0.47616300
H	-5.02524300	-0.00003500	0.95081000
H	-3.86662800	2.15299100	0.47622400
H	-1.57281900	2.14970800	-0.46070000

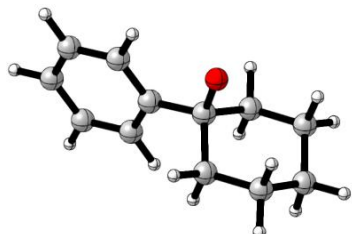
H	-3.86662800	2.15299100	0.47622400
H	-1.57281900	2.14970800	-0.46070000
C	4.71905100	-0.00002800	-0.33399700
H	4.79204000	0.88801200	-0.97144300
H	5.53918700	-0.00008400	0.38725500
H	4.79195600	-0.88804200	-0.97148800

1e-IM



C	1.56953500	-0.30064400	1.20749400
C	0.80387300	0.36156800	-0.00001000
C	1.56953900	-0.30071900	-1.20744200
C	3.04746100	-0.35126400	-0.77844100
C	3.04745200	-0.35149500	0.77845600
H	1.39173000	0.26343700	2.12799600
H	1.15012000	-1.30330700	1.34583200
H	1.15028600	-1.30347600	-1.34560900
H	1.39161900	0.26319400	-2.12802600
H	3.54214500	-1.23649800	-1.19437400
H	3.58281100	0.52416100	-1.15715100
H	3.54183300	-1.23703200	1.19410600
H	3.58311200	0.52361700	1.15745300
C	-0.70593100	0.11693400	0.00000000
C	-1.59358000	1.20081200	0.00012700
C	-1.23761500	-1.18296800	-0.00015200
C	-2.97645400	0.99264600	0.00011600
H	-1.19074100	2.20841000	0.00024000
C	-2.61829500	-1.39461300	-0.00016400
H	-0.57465900	-2.04527900	-0.00026500
C	-3.49514500	-0.30500100	-0.00002700
H	-3.64822700	1.84767600	0.00022000
H	-3.00804800	-2.40966400	-0.00028000
H	-4.57003400	-0.46720500	-0.00003600
O	1.14912600	1.68255300	0.00001700

1b-IM



C	0.99272400	0.12074200	-0.00008300
C	1.90965100	1.17999600	-0.00038700
C	1.48873900	-1.19291900	0.00035400
C	3.28632300	0.93442600	-0.00025100
H	1.53451300	2.19824400	-0.00072500

C	2.86348500	-1.44204000	0.00049200
H	0.80312500	-2.03703300	0.00059200
C	3.76959900	-0.37696400	0.00019100
H	3.98118900	1.77083800	-0.00049400
H	3.22546700	-2.46734600	0.00083600
H	4.83968500	-0.56835900	0.00029600
O	-0.81056300	1.74071100	-0.00078800
C	-0.51591300	0.40864400	-0.00026100
C	-1.20899700	-0.20910400	-1.27840100
C	-1.20896900	-0.20779500	1.27858900
C	-2.73249700	-0.05967800	-1.26529300
H	-0.93055600	-1.26953800	-1.30918400
H	-0.76533900	0.26930400	-2.15820700
C	-2.73247200	-0.05844000	1.26538000
H	-0.93047000	-1.26818300	1.31039300
H	-0.76528000	0.27151800	2.15788300
C	-3.34874600	-0.67335100	0.00035000
H	-3.14362500	-0.54288800	-2.16183600
H	-2.99470000	1.00352300	-1.32300300
H	-3.14353700	-0.54081600	2.16240300
H	-2.99472100	1.00480200	1.32208900
H	-4.43677500	-0.53029600	0.00029600
H	-3.17203400	-1.76056300	0.00088000