Supporting Information

Competing Pathways for Photoremovable Protecting Groups: The Effects of Solvent, Oxygen and Encapsulation

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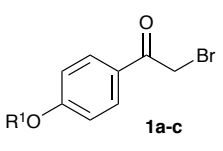
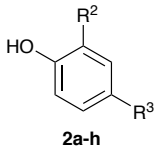
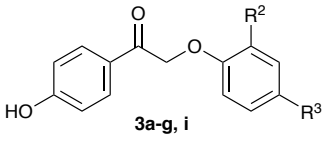


1a-c



2a-h

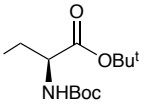


3a-g, i

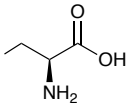
1a: R_1 = H
1b: R_1 = Ac
1c: R_1 = CO_2But

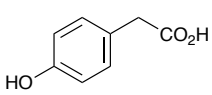
2a, 3a: R_2 = H; R_3 = CN
2b, 3b: R_2 = CF_3; R_3 = H
2c, 3c: R_2 = H; R_3 = CF_3
2d, 3d: R_2 = H; R_3 = H
2e, 3e: R_2 = H; R_3 = CH_3
2f, 3f: R_2 = H; R_3 = OCH_3
2g, 3g: R_2 = H; R_3 = Br

2h: R_2 = H; R_3 =



2i, 3i: R_2 = H; R_3 =





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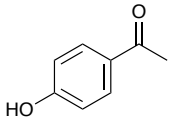

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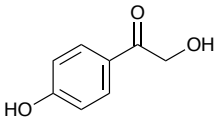

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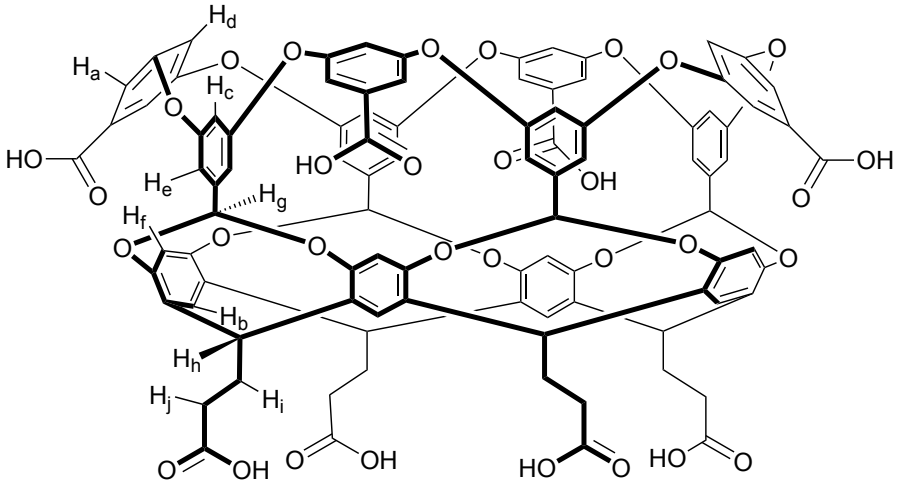


OA

Scheme 1. Structures of starting materials, intermediates, pHP triggers and octa acid (OA)[1] host.

2. Chemicals, Materials, and Equipment

2.1 Chemicals and Materials

Compounds di-*tert*-butyldicarbonate (DiBoc) and *t*-Boc protected ethyl tyrosyl esters, used for synthesis of pHP triggers, *p*-hydroxyacetophenone, *p*-cyanophenol, *o*-trifluoromethylphenol, *p*-methylphenol, *p*-bromophenol, *p*-hydroxyphenyl acetic acid, (*p*-hydroxybenzoyl)methanol, utilized for synthesis or for identification/quantification of triggers and photoproducts, potassium ferrioxalate, trifluoroacetic acid, 1,2,3-tribenzenetricarboxylic acid, phenanthroline, (Sigma-Aldrich/Alfa Aesar), utilized for determination of quantum yields, (Sigma-Aldrich/Alfa Aesar) were used as received.

Organic solvents acetonitrile, ether, dioxane, dichloromethane and ethyl acetate were p.a. grade and used as received while acetonitrile and formic acid used for chromatographic separations were HPLC gradient grade/LC-MS grade (VWR). TLC was carried out using 0.25 mm Merck silica gel plates (60F-254) and column chromatography was performed with 230-400 mesh Merck silica gel 60 for flash chromatography.

2.2 Equipment

The melting points of synthesized compounds were taken on a micro melting point apparatus. IR spectra were obtained in liquid films or KBr disks on an FT-IR spectrometer and their UV-vis spectra recorded on a Cary-100. The synthesized compounds were analyzed by NMR, using 400 MHz and 500 MHz Bruker instruments, and by mass spectrometry, using a Bruker Daltonics micro TOFQ II.

Formation of host-guest complexes with OA and photoproducts was studied by NMR, using 400 MHz and 500 MHz Bruker instruments or using a 500 MHz JEOL system equipped with a Royal HFX probe. The formation of products was also followed by UV-Visible absorbance, using a Cary-100. The identification and quantification of photoproducts was performed by HPLC, by LC-DAD-MS (liquid chromatography coupled to mass spectrometry), using a Agilent LC coupled

to a Bruker Daltonics HCT *ultra* mass spectrometer, and by UHPLC-HRMS (liquid chromatography coupled to high resolution mass spectrometry), using a Thermo Ultimate 3000 UHPLC coupled to a Orbitrap Elite mass spectrometer.

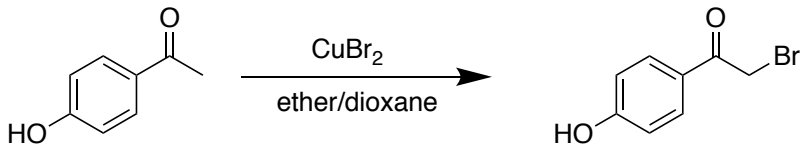
Irradiations were performed using two different setups. In one, a Rayonet RPR-100 merry-go-round photochemical reactor was used at 300 nm (RPR 3000 Å) or 350 nm (RPR 3500 Å). In the second the irradiations were performed using a high-pressure xenon lamp in conjunction with a water filter to prevent heating of the sample solution. An additional Pyrex filter was inserted to remove UV light below 300 nm.

3. Synthetic Procedures and Spectral Data for pHP Phenol Ethers

Compounds **1a**, and **3a** through **3i** were synthesized according to reported procedures.[2,3] Octa Acid (OA) host was synthesized following literature procedure.[1]

3.1 Preparation of α-Bromo-*p*-hydroxyacetophenone (1a) and Acetyl-protected (1b) and Boc-protected (1c) pHPs

3.1.1 Preparation of α-Bromo-*p*-hydroxyacetophenone (1a)[2]

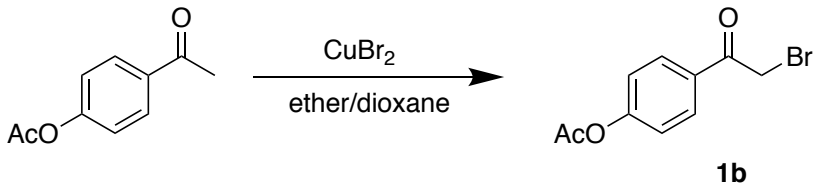


1a

To an ice-cooled solution of 2.06 g (15.1 mmol) of p-hydroxyacetophenone in 20 mL 1:1(ether/dioxane), was added a solution of 4.8 g (19.6 mmol, 1.3 equiv.) $CuBr_2$ in 20 mL of 1:1 ether/dioxane mixture in dropwise manner. After the addition, the solution was stirred at room temperature for 12 h, and the product was partitioned between water and EtOAc (2 x 20 mL). Combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated in vacuo.

The residue was purified by crystallization from CH_2Cl_2 to give **1a** as a colorless solid. Yield 1.9 g, (8.8 mmol, 58%), mp 126-128 °C/130 °C.

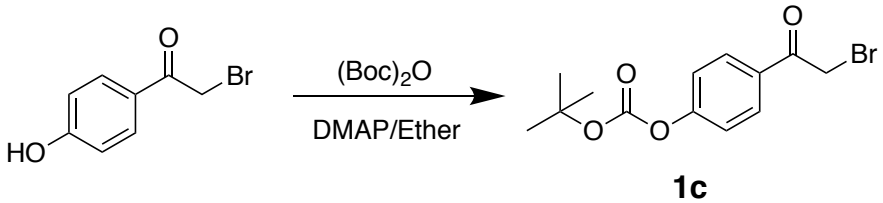
3.1.2 Preparation of α-Bromo-4'-acetoxyacetophenone (1b)



1b

To a solution of 5.6 g (32 mmol) of 4'-acetoxyacetophenone in 60 mL (1:1) dioxane/ether placed in an ice bath under nitrogen, was added 7.3 g (32 mmol) of $CuBr_2$ in 60 mL (1:1) dioxane/ether. The solution was stirred at room temperature for 4 h, then the solvent was removed *in vacuo*, and the product was partitioned between EtOAc and water. Organic phase was washed with 5% $NaHCO_3$ and brine, dried over Na_2SO_4, and concentrated *in vacuo* to give crude **α**-bromo-4'-acetoxyacetophenone (**1b**). The crude product was crystallized from (1:1) hexane/EtOAc to give the product **1b** as a colorless solid. Yield 7.1 g (27.6 mmol, 86%). ^{1}H NMR ($CDCl_3$) δ 2.35(s, 3H), 4.45 (s, 2H), 7.26 (d, J = 8.8 Hz, 2H), 8.03 (d, J = 8.8 Hz, 2H). ^{13}C NMR ($CDCl_3$) δ: 21.6, 31.1, 122.6, 131.9, 132.0, 155.4, 169.2, 191.7.

3.1.3 Preparation of BOC-Protected pHP Bromide (1c)



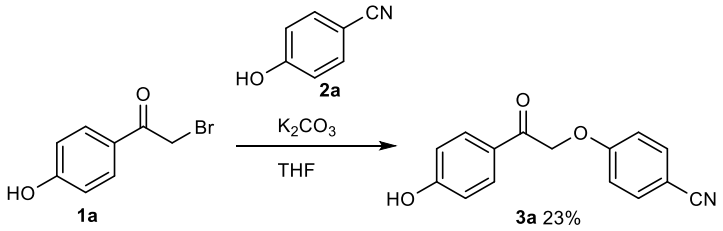
1c

To a solution of 10.0 g (46.5 mmol) α-bromo-*p*-hydroxyacetophenone (α-bromo-pHP) and catalytic amount of DMAP in 200 mL of anhydrous ether in an ice bath under nitrogen was added 11.1 g (50.8 mmol) di-tert-butyldicarbonate ($(Boc)_2O$) in 50 mL ether over 15 min. The reaction was stirred for 4 h at room temperature, then was washed twice with water (10 mL), saturated NaCl, dried over Na_2SO_4, and concentrated *in vacuo* to give 14.1 g of **1c** as a colorless solid, mp: 63.5-64.2 °C. Yield 14.1 g, (44.6 mmol, 96%). ^{1}H NMR ($CDCl_3$) δ: 1.57 (s, 9H), 4.43 (s, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 8.11(d, *J* = 8.4 Hz, 2H). ^{13}C NMR ($CDCl_3$) δ: 28.0, 31.1, 84.5, 121.8, 131.4, 130.8, 151.0, 155.4, 190.2. HRMS (ESI, m/z): Calcd. $(M+H)^+$ 296.0923, Found 296.0925

3.2 Synthesis of pHP Substituted Phenyl Ethers 3a, b, e, g and i

Preparation of 1-(4-hydroxyphenyl)-2-(4-(trifluoromethyl) phenoxy)ethan-1-one (**3c**, pHP *p*-trifluoromethylphenyl ether), 1-(4-hydroxyphenyl)-2-phenoxyethan-1-one (**3d**, pHP phenol ether), and 1-(4-hydroxyphenyl)-2-(4-methoxyphenoxy)ethan-1-one (**3f**, pHP *p*-ansyl ether) have been reported previously.[3]

3.2.1 Preparation of 4-(2-(4-Hydroxyphenyl)-2-oxoethoxy)benzonitrile (3a, pHP *p*-Cyanophenyl Ether)



Prepared using the same procedure employed for **3e** Yield (2.1g and 23%) (*vide infra*). pHP protected 4-cyanophenol displayed the following physical and spectral data: mp 224-225 °C as colorless crystalline needles. UV: 272 (ε 5940), 249 (ε 5900), 218 (ε 3800); IR (KBr), 3276 (OH), 2229 (CN), 1693 (C=O). ^{1}H NMR ($CDCl_3$) δ: 5.48 (s, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 7.12 (d, *J* = 8.8 Hz, 2H), 7.62 (d, *J* = 8.8 Hz, 2H), 7.92 (d, *J* = 8.8 Hz, 2H), 7.96 (s, OH). ^{13}C NMR ($CDCl_3$) δ: 68.5, 102.1, 114.2, 117.4, 124.2, 128.9, 132.4, 152.7, 160.2, 161.6, 189.8. HRMS (ESI, m/z): Theoretical (M+H) 254.0817, Found 254.0819.

3.2.2 Preparation of 1-(4-Hydroxyphenyl)-2-(2-(Trifluoromethyl)phenoxy)ethan-1-one (3b, pHP *o*-Trifluoromethylphenyl Ether)

To a solution of 0.93 g (5.7 mmol) *o*-trifluoromethylphenol and 1.48 g (5.7 mmol) of bromo ester **1b** in 50 mL acetone, 2 g of K_2CO_3, was added. The mixture was stirred for 12 h, then filtered. The filtrate was concentrated *in vacuo* and the crude product was eluted through silica gel column using 4:1 hexane:EtOAc as the mobile phase to purify. 4-(2-(2-(trifluoromethyl)phenoxy)acetyl)phenyl acetate was obtained as a white solid 0.77g (2.6 mmol, 46%). ^{1}H NMR ($CDCl_3$) δ: 2.34 (s, 3H), 5.32 (s, 2H), 6.89 (d, J = 8.8 Hz, 1H), 7.06 (t, J = 8.8 Hz, 1H), 7.24 (d, J = 8.8 Hz, 2H), 7.45 (t, J = 8.8 Hz, 1H), 7.61 (d, J = 8.8 Hz, 1H), 8.08 (d, J = 8.8 Hz, 2H). ^{13}C NMR ($CDCl_3$) δ: 14.60, 60.82, 113.31, 121.49, 119.56 (q, J = 32.4 Hz, 1C), 122.56, 127.80 (q, J = 5.2 Hz, 1C), 123.34 (q, J = 269 Hz, 1C) 130.4, 132.2, 133.7, 155.5, 169.2, 193.5. HRMS (ESI, m/z): Theoretical (M+ H) 339.0844, Found 339.0838.

To a solution of 0.90 g (2.7 mmol) 2'-(2-trifluoromethylphenoxy)-4-acetyloxyacetophenone in 30 mL methanol, was added the 1.5 g of KOH. The mixture was stirred for 12 h. The mixture was filtered, and the filtrate was concentrated *in vacuo*. The residue was purified by flash column with 3:1 hexane/EtOAc. 1-(4-hydroxyphenyl)-2-(2-(trifluoromethyl)phenoxy)ethan-1-one **(3b)** was obtained as colorless solid, m.p. 174-175 °C. Yield 0.69 g (2.3 mmol, 86%). The spectral data were as follows: ^{1}H NMR ($CDCl_3$/DMSO) δ 5.31 (s, 2H), 6.83 (m, 3H), 6.96 (t, J = 8.8 Hz, 1H), 7.38 (t, J = 8.8 Hz, 1H), 7.49 (d, J = 8.8 Hz, 1H), 7.83 (d, J = 8.8 Hz, 2H), 10.06 (s, OH); ^{13}C NMR ($CDCl_3$/ DMSO) δ 70.4, 112.6, 115.3, 118.1 (q, J = 30.6 Hz, 1C), 120.2, 122.1, 123.2 (q, J = 270 Hz, 1C), 125.4, 126.6, 130.2, 132.9, 155.6, 162.6, 191.5. (ESI, m/z): Calcd. $(M+H)^+$ 297.0739, Found 297.0753.

3.2.3 Preparation of 1-(4-Hydroxyphenyl)-2-(*p*-tolyloxy)ethan-1-one (3e, pHP *p*-Toluyl Ether)

To a cooled (ice bath) solution of 1.18 g (11 mmol) of 4-methylphenol in 20 mL of THF, was added 0.36 g (60% in mineral oil) NaH slowly. To this mixture, the solution of 1.8 g (8.7 mmol) of α-bromo-*p*-hydroxyacetophenone in 20 mL of THF was added drop wise through an

additional funnel. After 2 h, the white solid was filtered and the remaining solution of the filtrate was stirred with a magnetic stir bar at room temperature for an additional 24h. The mixture was filtered and the filtrate was concentrated using a rotary evaporator. Flash column was used to separate the mixture by using 3:1 hexane/EtOAc to obtain the product **3e** as colorless needles, mp 154-156 ^{o}C. Yield, 0.80 g (2.6 mmol, 30%). UV ε_{271}=18000, ε_{218}=19000. IR, 3211(OH), 1664 (C=O). ^{1}H NMR ($CDCl_3$) δ: 2.30 (s, 3H), 5.21 (s, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 7.10 (d, *J* = 8.8 Hz, 2H), 7.99 (d, *J* = 8.8 Hz, 2H). ^{13}C NMR ($CDCl_3$) δ: 20.70, 71.15,114.86, 115.79, 128.12, 130.22, 131.11, 156.17, 160.71, 193.58. HRMS (ESI, m/z): Calcd. $(M+H)^+$ 243.1021, Found 243.1024.

3.2.4 Preparation of 2-(4-Bromophenoxy)-1-(4-hydroxyphenyl)ethan-1-one (3g, pHP *p*-Bromophenyl ether)

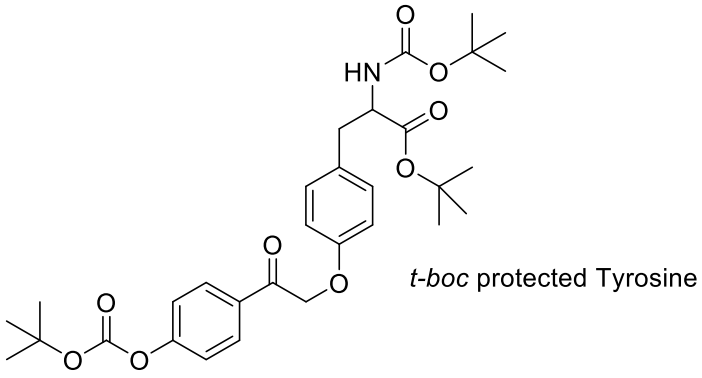
To an ice-cold solution of 0.55 g (3.2 mmol) of *p*-bromophenol (**2 g**) and 0.59 g (4.3 mmol) of K_2CO_3 in 20 mL of acetone, 0.45 g (2.1 mmol) of **1a** was added drop wise using an addition funnel. After 2 h, the white solid was filtered and the remaining filtrate was stirred at room temperature for an additional 24h. The resulting mixture was filtered and the filtrate was concentrated *in vacuo*. The mixture was purified by flash chromatography by using 3:1 hexane/EtOAc as the mobile phase to obtain the product as a colorless solid. Yield 0.30 g (0.59 mmol, 28%). Upon heating, the solid decomposed before the melting point was reached. UV: 272 (ε 940), 249 (ε 5900), 218 (ε 3800). IR (KBr), 3276 (OH), 2229 (CN), 1693 (C=O). ^{1}H NMR ($CDCl_3$) δ: 5.48 (s, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 7.12 (d, *J* = 8.8 Hz, 2H), 7.62 (d, *J* = 8.8 Hz, 2H), 7.92 (d, *J* = 8.8 Hz, 2H), 7.96(s, OH). ^{13}C NMR ($CDCl_3$) δ: 69.7, 112.5, 115.4, 130.0, 131.6, 156.9, 162.6, 191.5. HRMS (ESI, m/z): Calcd. $(M+H)^+$ 328.9789, Found 328.9805.

3.2.5 Preparation of Protected pHP Tyrosyl Ethyl Ester, R = Et and pHP Tyrosyl Ether (3i)

The general method of Frechet, et al.[4] was employed to protect the amino acid moieties on the peptide. For the tyrosyl pHP derivative, it was necessary to first protect the amino acid functional groups. Using the sequence reported by Frechet.[4] The model ethyl ester of tyrosine was

first employed to protect both the amino and the pHP phenolic group. Then, selective removal of the *t*-butyl group on tyrosine and installation of *t*-Boc protected pHP bromide was carried out. Finally, the *N*-*t*-butyl group was removed yielding the pHP tyrosyl ethyl ester. This same sequence was repeated with tyrosine in which all the functional groups were protected with *t*-Boc, the phenol groups was deprotected, and the pHP group was installed. These procedures were then repeated on tyrosine to yield the desired final pHP tyrosine (**3i**).

3.2.6 Synthesis of t-Boc Protected pHP Tyrosine (3i)



t-boc protected Tyrosine

To a solution of 1.45 g (5.6 mmol) of α-bromo-4'-*t*-butoxyacetophenone (**1c**) and 1.9 g (5.6 mmol) of *t*-Boc protected tyrosine in 20 mL of acetone was added 1.0 g (7.4 mmol) potassium carbonate and a catalytic amount of KI. The mixture was refluxed at 60 ^{o}C for 24 h, the solid was filtered, and the filtrate was concentrated *in vacuo*. Flash column chromatography was used to separate the mixture with a 7:3 hexane/EtOAc to obtain *t*-Boc protected pHP *t*-butyl tyrosine ester as a colorless solid, mp 90-92 ^{o}C. Yield 2.89 g, (4.87 mmol, 87%). UV ε_{228} = 12000, ε_{247} = 13000. ^{1}H NMR ($CDCl_3$) δ: 1.41 (s, 9H), 1.44 (s, 9H), 1.59 (s, 9H), 3.01 (d, *J* = 5.6 Hz, 2H), 4.41 (q, *J* = 8.0 Hz, 1H), 4.98 (*d*, *J* = 7.60 Hz, 1H), 5.22 (s, 2H), 6.87 (d, *J* = 8.4 Hz, 2H), 7.10 (t, *J* = 8.4 Hz, 2H), 7.32 (*d*, *J* = 8.4 Hz, 2H), 8.06 (d, *J* = 8.4 Hz, 2H), 7.48 (t, *J* = 8.8 Hz, 1H), 7.89 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR ($CDCl_3$) δ: 28.1, 28.4, 28.7, 84.5, 82.4, 80.1, 71.4, 55.3, 38.0, 115.0, 122.0, 130.0, 130.3, 131.1, 132.4, 151.3, 155.5, 155.6, 157.4, 171.4, 193.8. HRMS (ESI, m/z): Calcd. $(M+H)^+$ 594.2679, Found 594.2691.

A solution of 0.50 g (0.87 mmol) of the *t*-Boc protected pHP *t*-butyl tyrosine ester in 2 mL of TFA in 20 mL of CH_2Cl_2 was stirred for 60 min at room temperature. Then TFA solution was removed *in vacuo*. A white solid of pHP tyrosine **3i** was obtained: ^{1}H NMR (DMSO-d_6) δ: 3.17 (m, 2H), 4.12 (m, 1H), 5.38 (s, 2H), 6.91 (d, J = 8.4 Hz, 2H), 6.96 (d, J = 8.4 Hz, 2H), 7.19 (*d*, J = 8.4 Hz, 2H), 7.92 (d, J = 8.4 Hz, 2H). ^{13}C NMR (DMSO-d_6) δ: 34.8, 53.5, 69.5, 114.4, 115.1, 125.8, 126.6, 130.0, 130.3, 157.3, 162.7, 169.4, 192.2. HRMS (ESI, m/z): Calcd. $(M+H)^+$ 316.1185, Found 316.1181.

4. Photolysis Procedures and Quantum Yield Determination in Solution

4.1 Photolysis of pHP Triggers 3a-g

Photolysis of pHP phenol ethers **3a–g** were carried out in a Rayonet RPR-100 photochemical reactor using 300 nm (RPR 3000 Å) or 350 nm (RPR 3500 Å) lamps fitted with an RPR merry-go-round apparatus. The experiments were carried out using NMR tubes or 20 × 180 mm Pyrex test tubes with samples of 20 – 100 mg of the ethers dissolved in appropriate solvents (2 – 5 mL) with internal standards of either 1,2,3-benzenetricarboxylic acid or DMF. The pH was adjusted with either Tris or phosphate buffer solution by addition of TFA, HCl and NaOH. For 300 nm irradiations, the reactor was fitted with only 4 or 8 lamps and turned on before sample placement to warm up the lamps for 15 min prior to removing an opaque sleeve to start the photolysis. A counter recorded the time of irradiation. The light output for the determination of quantum efficiencies was measured using potassium ferrioxalate, *vide infra*.[1] Photolysis times ranged up to 10 hours, depending on the conversion desired, the efficiency of the reaction, and the size of the sample. The progress of the reaction was monitored by ^{1}H NMR. Product yields were determined by ^{1}H NMR using DMF as the internal standard. After completion of the photolysis, the products were isolated by HPLC or standard flash column chromatography. Compounds **3c** and **3f** were also irradiated in mixtures D_2O:acetonitrile-d_3 20:80 using a high-pressure xenon lamp in conjunction with water and Pyrex filters. Figures S1 and S2 show the ^{1}H NMR obtained for these compounds before and after irradiation.

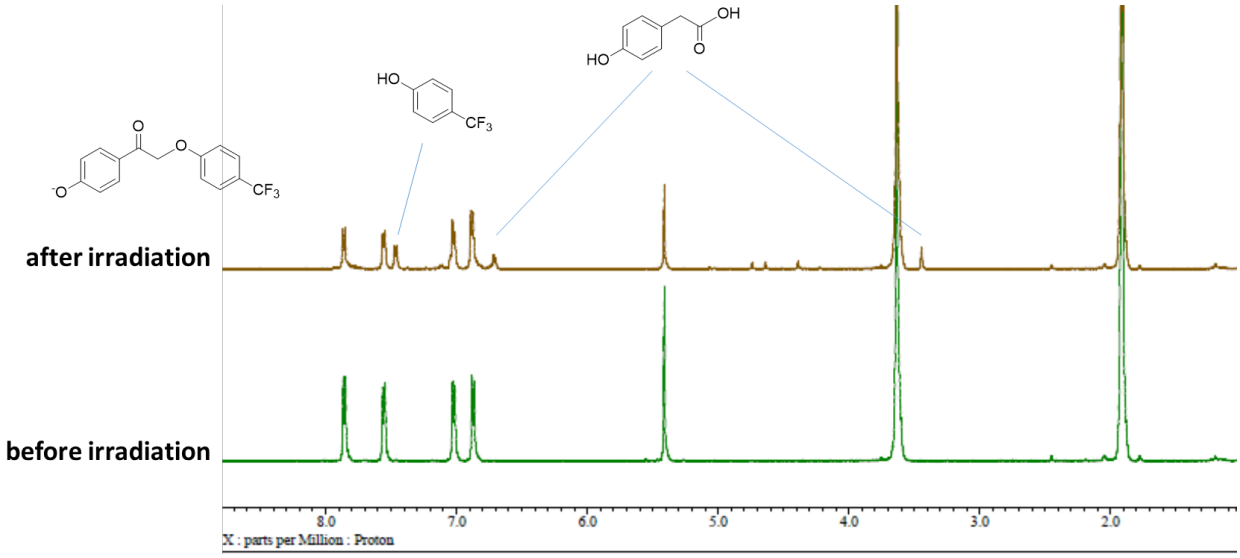


Figure S1. ^{1}H NMR spectra of **3c** in D_2O:acetonitrile-d_3 20:80 before and after irradiation.

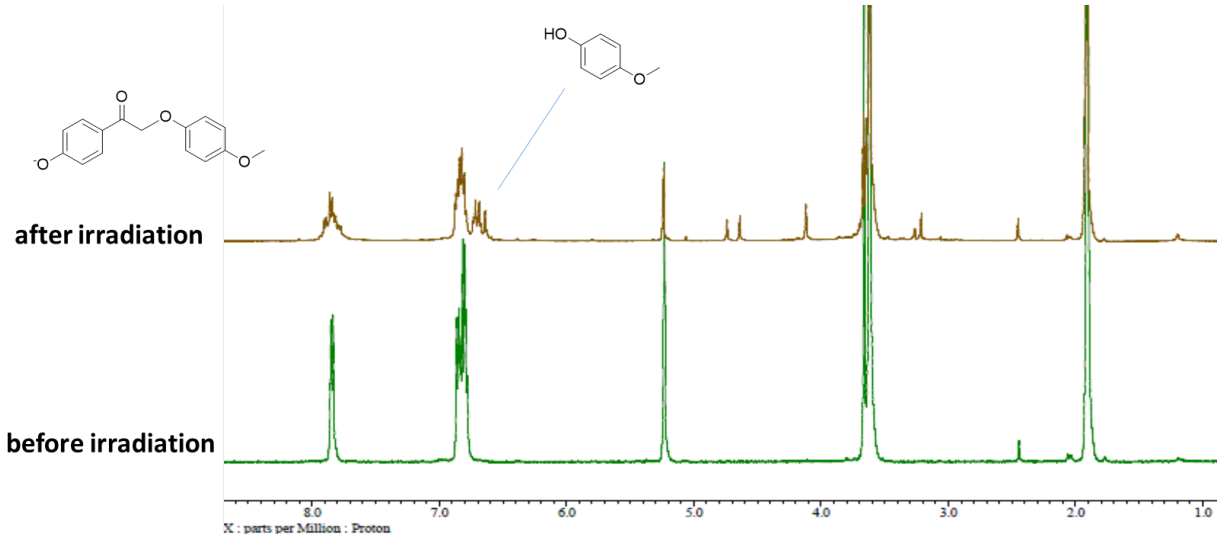


Figure S2. ^{1}H NMR spectra of **3f** in D_2O:acetonitrile-d_3 20:80 before and after irradiation.

Additional monitoring of the reaction by UV-vis spectroscopic analysis was accomplished by the following general procedures with ether **3b**. A 5 mg sample of 2,4-cyanophenoxy-4-hydroxyacetophenone was dissolved in 5 mL of 20% aqueous acetonitrile, buffered at pH 7.4 with a phosphate buffer, and the solution transferred to a Pyrex test tube. The sample was irradiated with eight 300 nm lamps and samples were periodically removed in 50 µL aliquots and diluted to

2 mL for UV analysis. The UV-vis spectra were recorded every 3 min of irradiation. The phototransformation of ethers **3c** and **3f** was also studied in dry acetonitrile and mixtures of acetonitrile:water 20:80 and 80:20. In this case, the irradiations were performed using a high-pressure xenon lamp in conjunction with water and Pyrex filters. Figures S3-S6 show the UV spectra before and after irradiation of **3c** and **3f** in dry acetonitrile and acetonitrile:water 20:80.

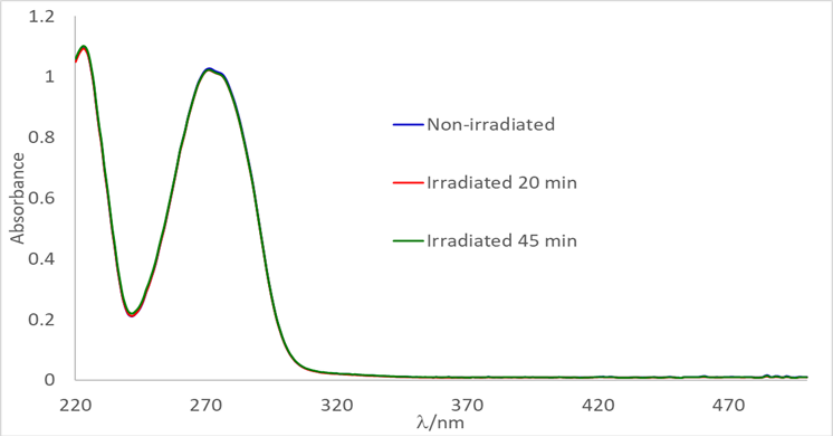


Figure S3. UV-vis traces obtained before and after photolysis of **3c** in dry CH_3CN. [**3c**] ~ 50 μM.

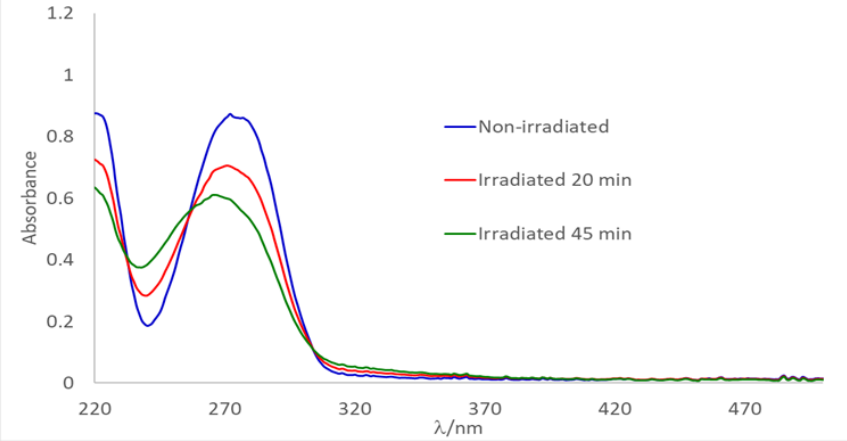


Figure S4. UV-vis traces obtained before and after photolysis of **3f** in dry CH_3CN. [**3f**] ~ 50 μM.

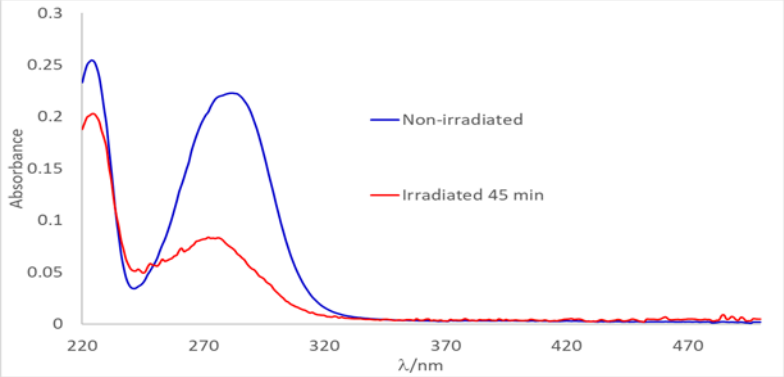


Figure S5. UV-vis traces obtained before and after photolysis of **3c** in water:acetonitrile mixture (80:20). [**3c**] ~ 12 μM.

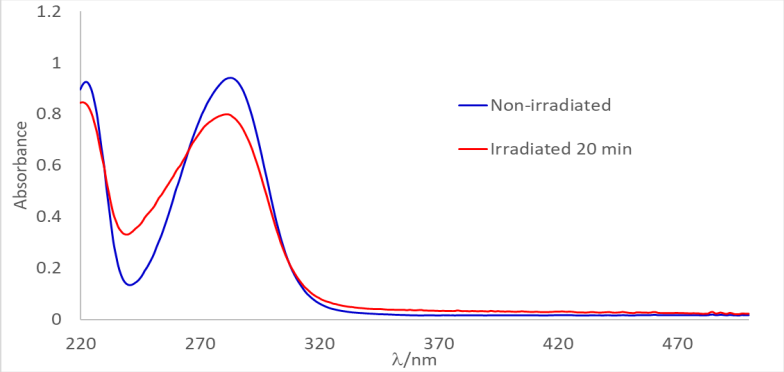


Figure S6. UV-vis traces obtained before and after photolysis of **3f** in water:acetonitrile mixture (80:20). [**3f**] ~ 50 μM.

4.2 Photolysis of pHP Tyrosyl Ether 3i

A 4 mM solution of pHP caged tyrosine **3i** was dissolved in 30% aqueous phosphate buffer (pH ~7.0)/CH_3CN was photolyzed at 300 nm. The initial optical density of the sample solution was >4.0 over the emission range of the 300 nm RPR lamps, assuring the complete absorption by the sample for quantum yield measurements at low conversions. Higher conversion (1 hour photolysis) gave 82%, released tyrosine at 80% conversion.

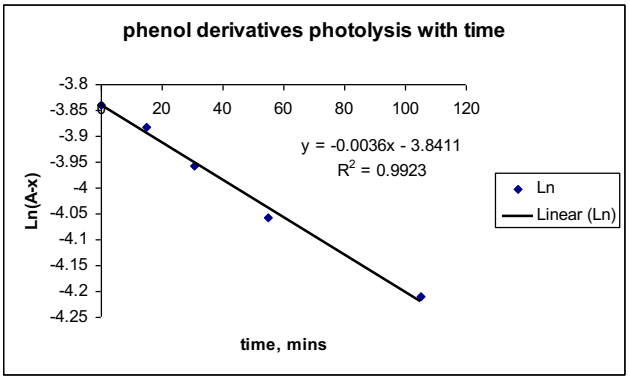
The quantum yield determinations gave $\Phi_{dis} = 0.1$ for pHP tyrosine disappearance and $\Phi_{app} = 0.085$ for the appearance of uncaged tyrosine. Stern-Volmer quenching constants (K_{SV}) were carried out using methyl sorbate. Light output was determined using potassium ferrioxalate method of Parker and Hatchard.[1] See quenching studies below for details.

4.3 Actinometry

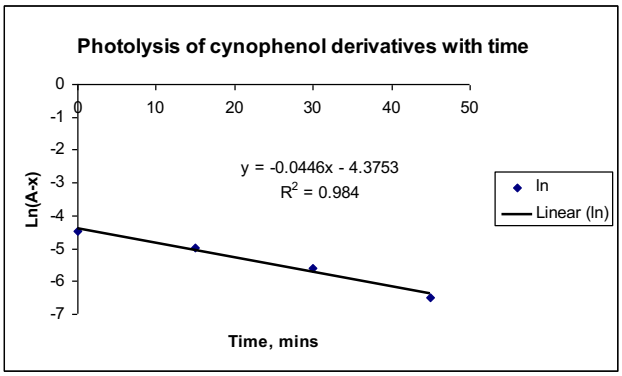
A solution of 0.6 mM of potassium ferrioxalate in 0.05 M H_2SO_4 was irradiated under identical conditions as the pHP ethers, i.e., with the same lamps, test tubes, and volumes. The procedure of preparation and handling of actinometer as well as calibration curve are detailed by Hatchard and Packer.[5] To a 10 mL volumetric flask was added 0.5 mL buffer, 2 mL 0.1% phenanthroline, 0.9 mL 0.05 M sulfuric acid, and 0.1mL of the irradiated solution. Absorbance was recorded. The difference in optical density was converted to concentration using a calibration curve. The change in concentration was converted to mol/min and light output was determined by dividing this number by 1.24.[5] The optical density was measured at 510 nm.

4.4 Quantum Yield Determination

Quantum yields of ether disappearance, Φ_{dis} (**3a** – **f**, **i**), and product appearance, Φ_{ArOH} (**2a** – **f**, **i**) were determined by reverse phase HPLC using the internal standard method. The quantum yields for photorearrangement product of pHP cage, *p*-hydroxyphenylacetic acid (**4**) along with *p*-hydroxyacetophenone (**5**) and 2',4-dihydroxyacetophenone (**6**) were determined by the relative percentages of the differences between Φ_{ArOH} from Φ_{dis}. Figures S7a-b show the photolysis of **3a** and **3d** vs time. Note the extended time necessary for release of the unsubstituted phenol vs. that for *p*-cyanophenyl analog.



(a)



(b)

Figure S7. Photolysis of pHP phenyl ether **3d** (a) and *p*-cyanophenyl ether **3a** (b) in CH_3CN/H_2O.

4.5 Quenching Experiments

The Stern-Volmer expression for quenching of the release of *p*-cyanophenol from pHP *p*-cynophenol ether **3a** with methyl sorbate is $\Phi_0 / \Phi = 1 + K\text{sv}\,[Q]$. Photolysis at 310 nm gave *K*sv = 105.5 for the Stern-Volmer slope in the equation $\Phi_0 / \Phi = 1 + k_q\tau^3\,[Q]$ and τ^0, the lifetime of the excited triplet state in the absence of the quencher Q (methyl sorbate) is obtained for this reaction when $k_q = k_d$. Therefore, the lifetime $\tau^3 = k\text{sv}/k\text{d} = 4.2 \times 10^{-9}$ s or τ^0 4.2 ns, the lifetime of the reactive excited triplet state. Figures S8 and S9 show the Stern-Volmer plots for the quenching of the photoreaction of **3a** by methyl sorbate.

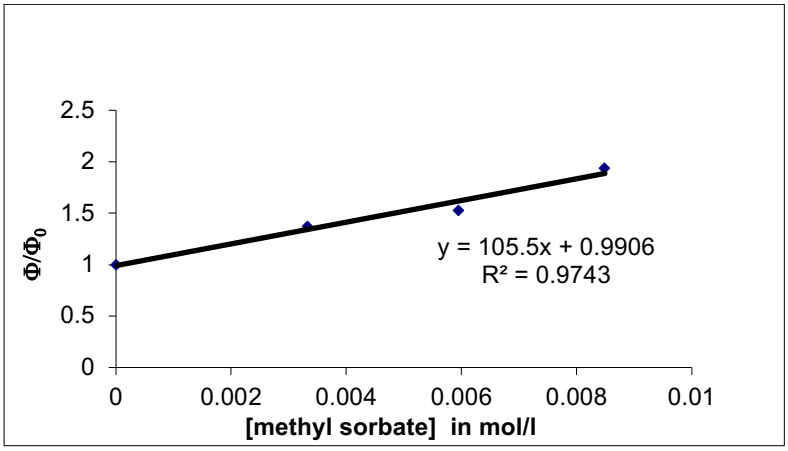


Figure S8. Stern-Volmer quenching by methyl sorbate of pHP *p*-cyanophenyl ether (**3a**) photolysis at 320 nm.

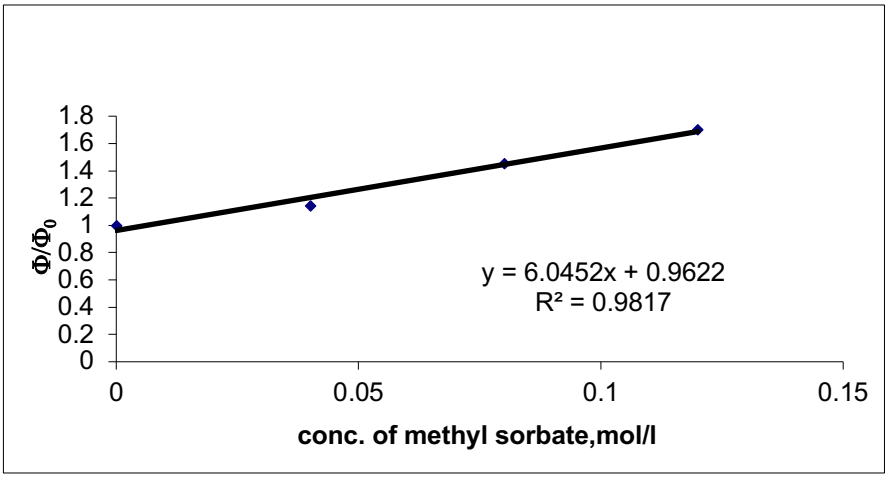


Figure S9. Stern-Volmer quenching by methyl sorbate of **3a** photolysis at 350 nm.

For photolysis at 350 nm, methyl sorbate quenching gave a Stern-Volmer quenching constant of *K*sv = 6.045 for $\Phi_0 / \Phi = 1 + k_q\tau^3$ [Q]. The τ^3 (the lifetime of the triplet in the absence of quencher Q) obtained was $k_q = k_d$, $\tau^3 = k_{sv}/k_d = 0.24$ ns.

5. pH Effect on Photochemistry of pHP Phenyl Ethers

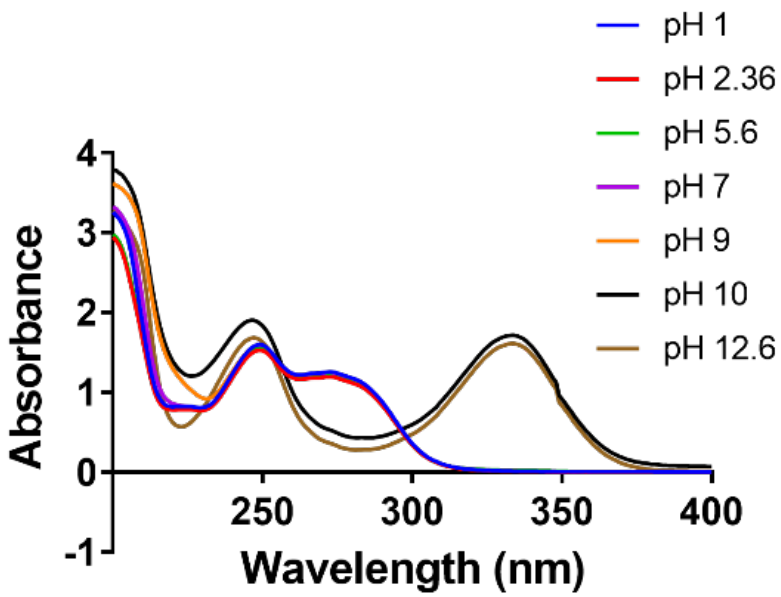


Figure S10. UV-vis spectrum of pHP *p*-cyanophenyl ether (**3a**) as a function of pH. The UV-vis spectra were measured for solutions of **3a** at pH 1.0 (aq. HCl) and over a range of pH from 2.4 to 12.8 in aq. phosphate buffer solutions (2.1×10^{-4} mol/L in $NaOD/D_2O$).

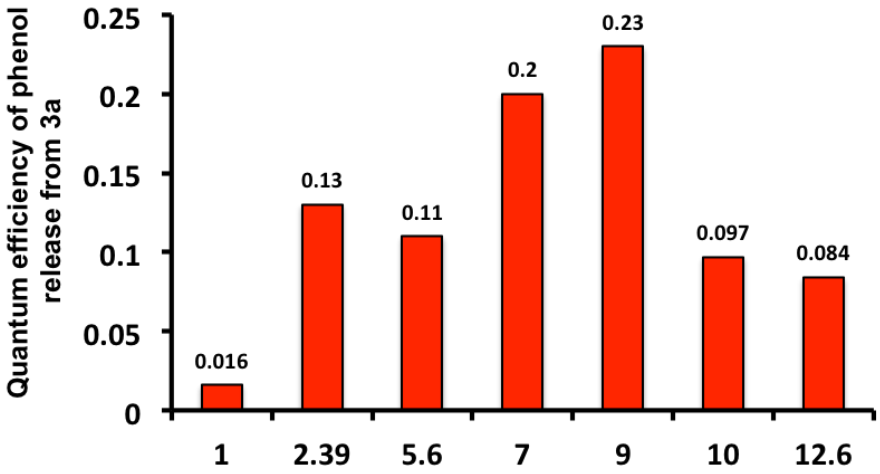


Figure S11. Effect of pH on the quantum efficiency of phenol release from pHP *p*-cyanophenyl ether (**3a**). pHP Cyanophenol ether **1a** (4.2×10^{-3} mol in 20% aq. CH_3CN) with 0.0275 g of biphenyl is used as the internal standard.

6. Supramolecular Encapsulation and Photochemistry of pHP Phenyl Ethers 3c and 3f

6.1 Photolysis of OA Enclosed 1-(4-Hydroxyphenyl)-2-(4-(trifluoromethyl) phenoxy)ethan-1-one (3c)

^{1}H NMR titration experiment: A 1 mM solution of OA in borate buffer (pH = 8.7) placed in a Pyrex NMR tube to which was added 2.5 μL of a 60 mM of **3c** in DMSO-d_6. ^{1}H NMR was employed to assure that the pHP ether (**3c**) forms a 1:2 complex with OA (**3c**:OA). See Figure S13.

UV-light irradiation experiment (monitored by ^{1}H NMR): A 1 mM solution of OA in borate buffer (pH = 8.7) was prepared in a Pyrex NMR tube after which a solution of 5 μL of a 60 mM solution of **3c** in DMSO-d_6 was added. The ^{1}H NMR spectra were recorded before and after the addition of **3c** to OA to form 1:2 complex **3c**@(OA)$_2$. The solution was then irradiated for 1 h using a 450 W medium pressure mercury lamp with Pyrex jacket. The ^{1}H NMR spectra showed a new peak at 3.3 ppm assigned to the methylene group of 4-hydroxyphenylacetic acid (**4**), the Favorskii rearrangement product. In addition, proton peaks of *p*-trifluorophenol (**2c**) and 2', 4-dihydroxyacetophenone (**6**) were also observed (See Figure 3 in the text). The photoreaction was also monitored by LC UV-vis. The phenol yield decreased if irradiation continued beyond 1 hr reflecting the instabilty of the phenol to the photolysis conditions.

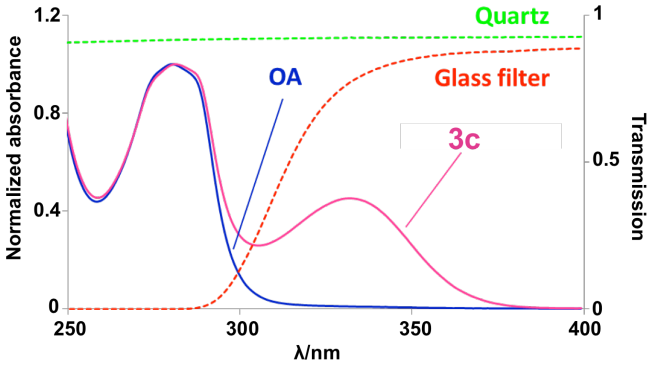


Figure S12. UV-vis spectra as a function of supramolecular encapsulation. Absorption spectra of **3c** in OA capsule (purple trace) and OA alone (blue trace) were dissolved in aqueous borate buffer (pH 8.7). The dotted red and green lines are the transmission profiles of Pyrex and quartz glass filters, respectively.

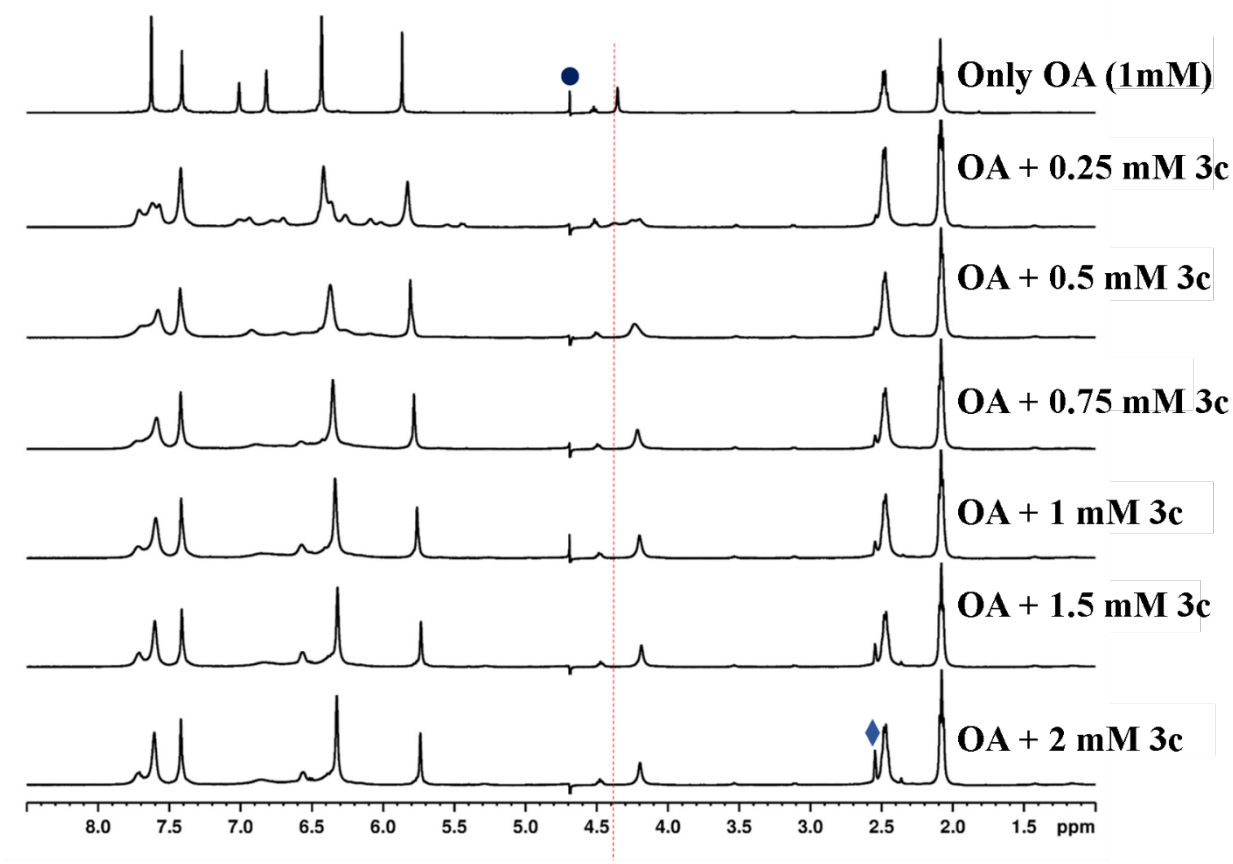


Figure S13. ^{1}H NMR titration spectra of **3c**@OA in borate buffer solution. The "●" and "◆" represent the residual solvent peaks for D_2O and DMSO-d_6, respectively.

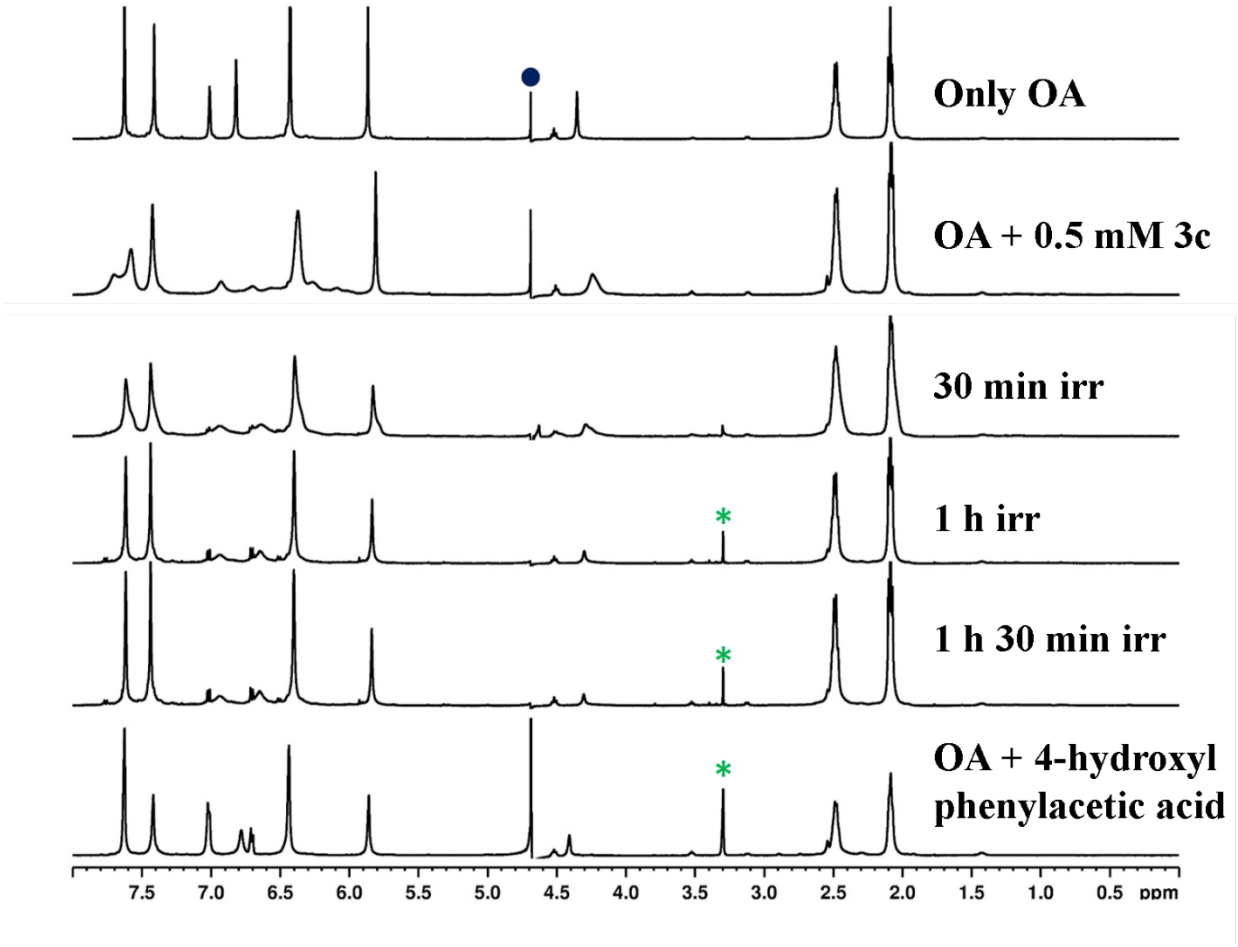


Figure S14. ^{1}H NMR spectra of **3c**@$(OA)_2$ in borate buffer solution(before and after irradiation). The "*" indicates the aliphatic proton signals of 4-hydroxyphenylacetic acid and "●" represents the residual solvent peak for D_2O.

The reaction of **3c** was ca. 32 times more efficient vis-à-vis **3f** (*p*-methoxyphenol release, *vide infra*). However, with respect to carboxylate, the release of all phenols was significantly slower.

6.2 Photolysis of OA Enclosed 1-(4-Hydroxyphenyl)-2-(4-methoxyphenoxy)ethan-1-one (3f)

^{1}H NMR titration experiment: A 1 mM solution of OA in borate buffer (pH = 8.7) was prepared in a Pyrex NMR tube after which a solution of 2.5 μL of a 60 mM solution of **3f** in DMSO-d_6 was added incrementally. The ^{1}H NMR spectrum was recorded after each portion. The upfield shift of the -OMe protons in **3f** indicated that the guest molecule was forming a complex with OA. This observation was accompanied by the disappearance of the guest OMe signal at -0.8 ppm. Further increase of **3f** concentration indicated that the excess guests did not enter the complex except by exchange with the fully complexed guest (the NMR titration experiment suggests that **3f** forms a 2:1 complex with OA (**3f**@$(OA)_2$). See Figures S15 ans S16 for **3f** irradiations.

UV-light irradiation experiment (monitored by ^{1}H NMR): A 1 mM solution of OA in borate buffer (pH = 8.7) was prepared in a Pyrex NMR tube after which a solution of 5 μL of a 60 mM solution of **3f** in DMSO-d_6 was added. The ^{1}H NMR spectra were recorded before and after the addition of **3f** to OA to form 1:2 complex **3f**@$(OA)_2$. The solution was then irradiated for 1 h using a 450 W medium pressure mercury lamp with Pyrex jacket. The ^{1}H NMR spectra showed a new peak at 3.3 ppm assigned to the methylene group of 4-hydroxyphenylacetic acid (**4**), the Favorskii rearrangement product. In addition, ^{1}H NMR absorptions were assigned to *p*-methoxyphenol (**2f**) and 2',4-dihydroxyacetophenone (**6**) were observed. The photoreaction was also monitored by LC UV-vis. The phenol yield decreased if irradiation continued beyond 1 hr reflecting the instabilty of the phenol to the photolysis conditions.

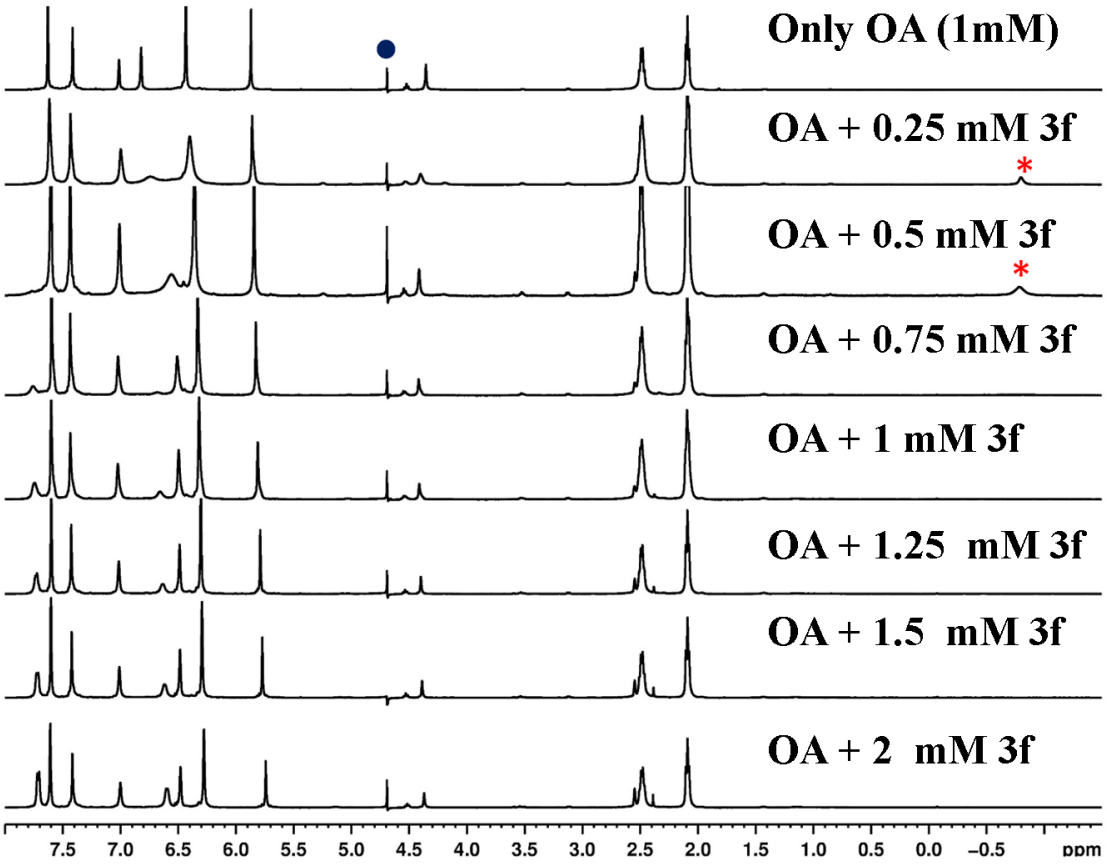


Figure S15. ^{1}H NMR titration spectra of **3f**@OA in borate buffer solution. "*" indicates the –OMe proton signals of **3f** are inside the OA cavity. The "●" represents the residual solvent peak for D_2O. A 2:1 OA:**3f** complex formed.

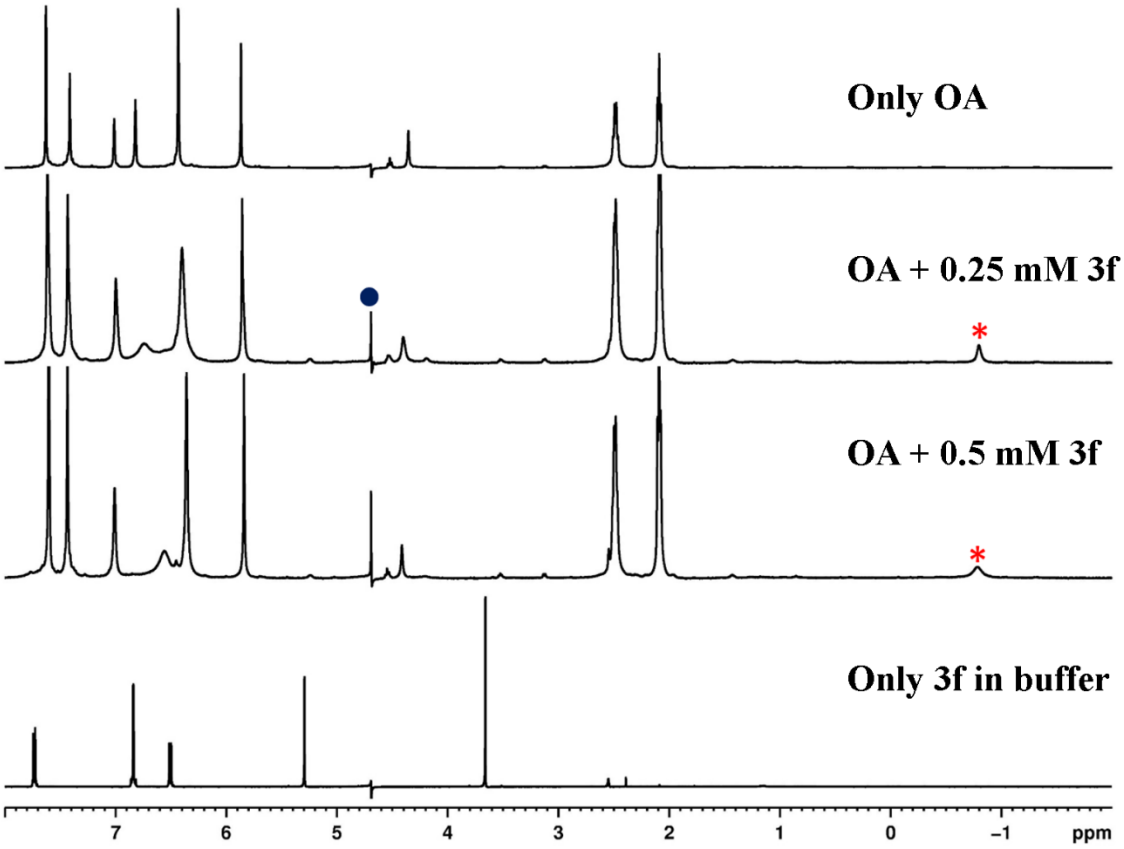


Figure S16. ^{1}H NMR titration spectra of **3f**@OA in borate buffer solution. "*" indicates the –OMe proton signals of **3f** are initially inside OA cavity. The "●" represents the residual solvent peak for D_2O. [OA] = 1 mM.

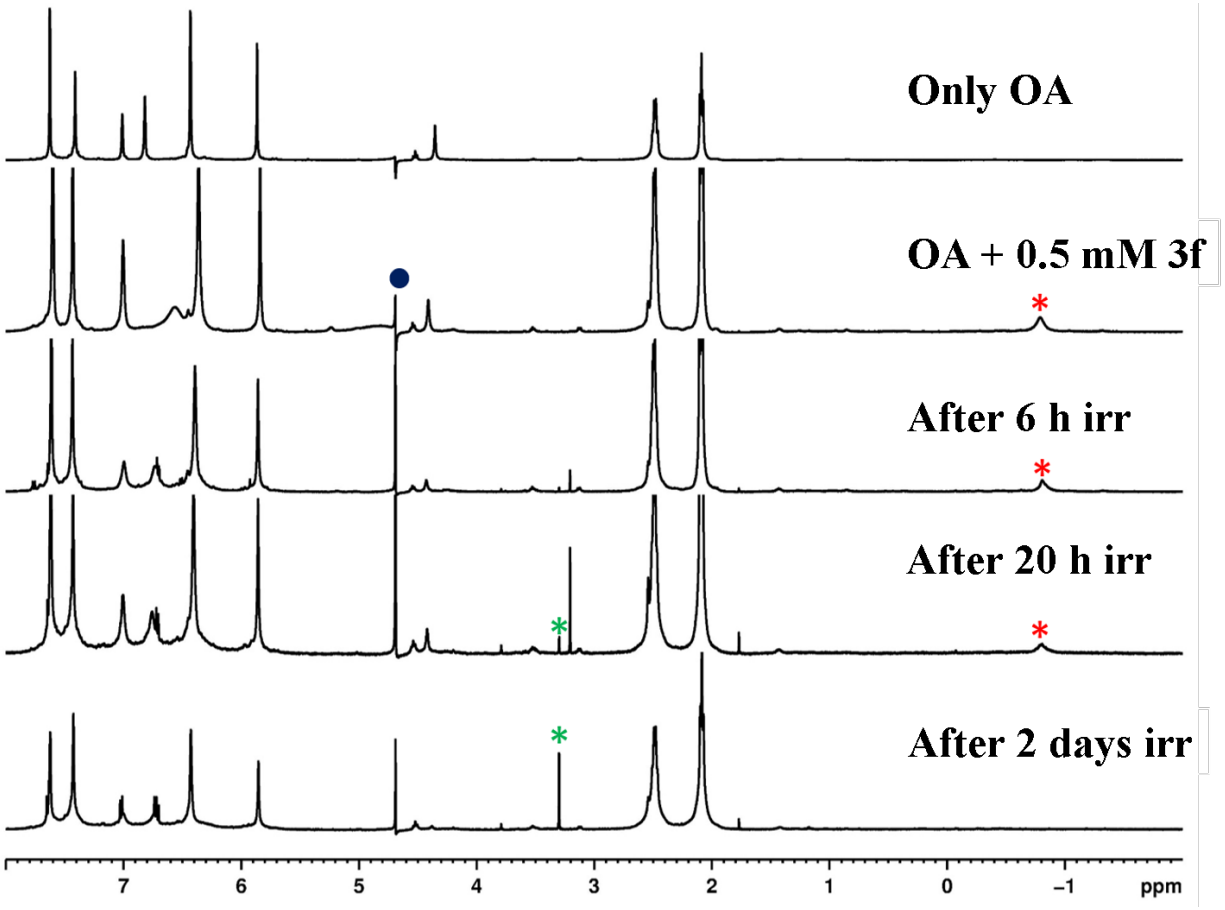


Figure S17. ^{1}H NMR spectra of **3f**@$(OA)_2$ in borate buffer solution (before and after irradiation). The "*" and "*" indicate the aliphatic proton peaks of **3f** are inside the OA cavity and 4-hydroxyphenylacetic acid, respectively **(4)**, respectively. The "●" represents the residual solvent peak for D_2O. [OA] = 1 mM.

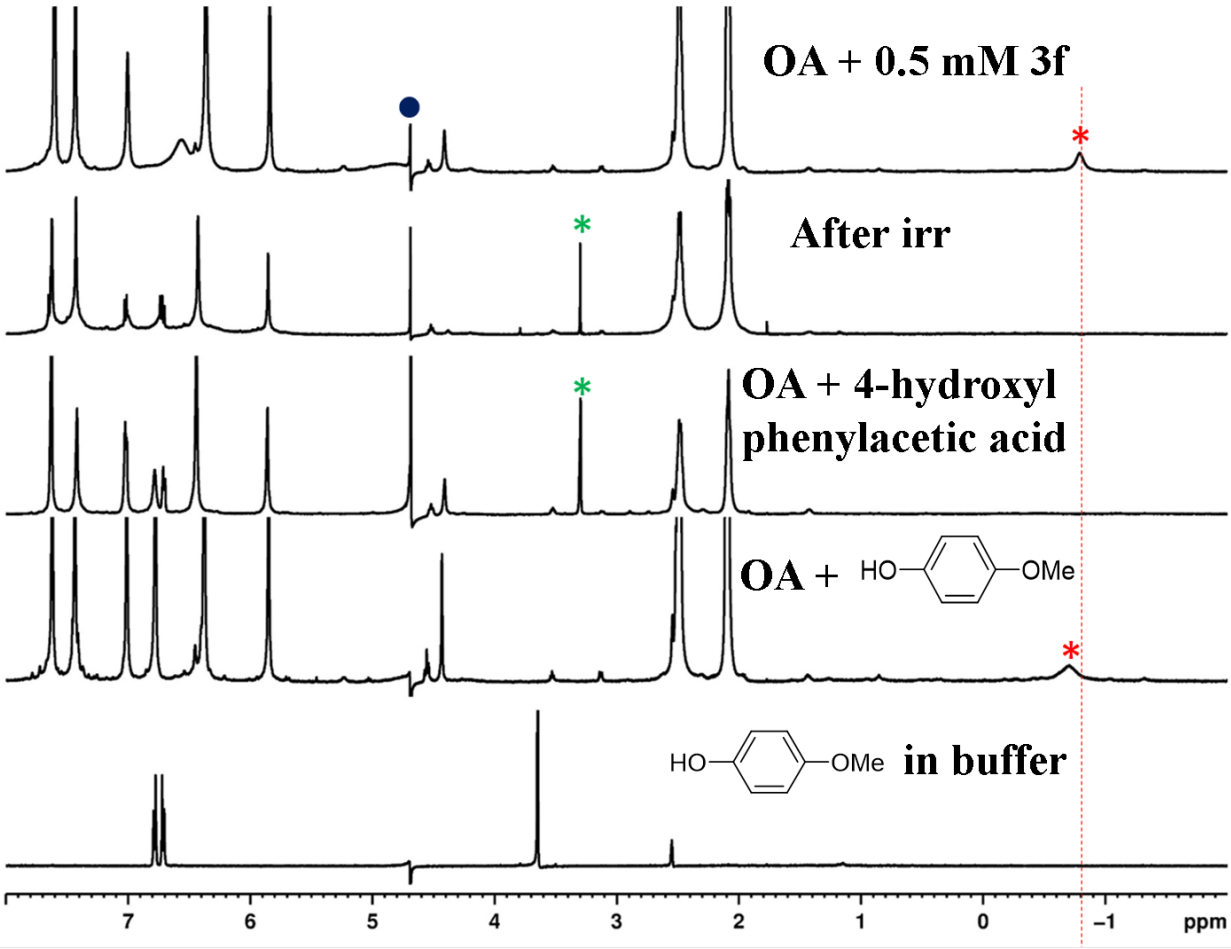


Figure S18. ^{1}H NMR spectra of **3f@**$(OA)_2$ in borate buffer solution (before and after irradiation). The "*" and "*" indicate the aliphatic proton signals of **3f** inside the OA cavity and 4-hydroxyphenylacetic acid **(4)**, respectively. "●" represents the residual solvent peak for D_2O, [OA] = 1 mM.

6.3 2D-NOESY Analysis of 3f@$(OA)_2$

About 5 mM solution of Octa Acid (OA) in borate buffer (pH = 8.7) was prepared in an NMR tube. To this solution, 25 μL of a 60 mM solution of **3f** in DMSO-d_6 was added and the 2D-NOESY spectrum recorded. The correlation peak corresponding to the methyl protons of **3f** and 'g' protons of OA indicate the complex formation. This also suggests that the guest molecule methyl protons are closer to the 'g' proton of OA (Figure S19).

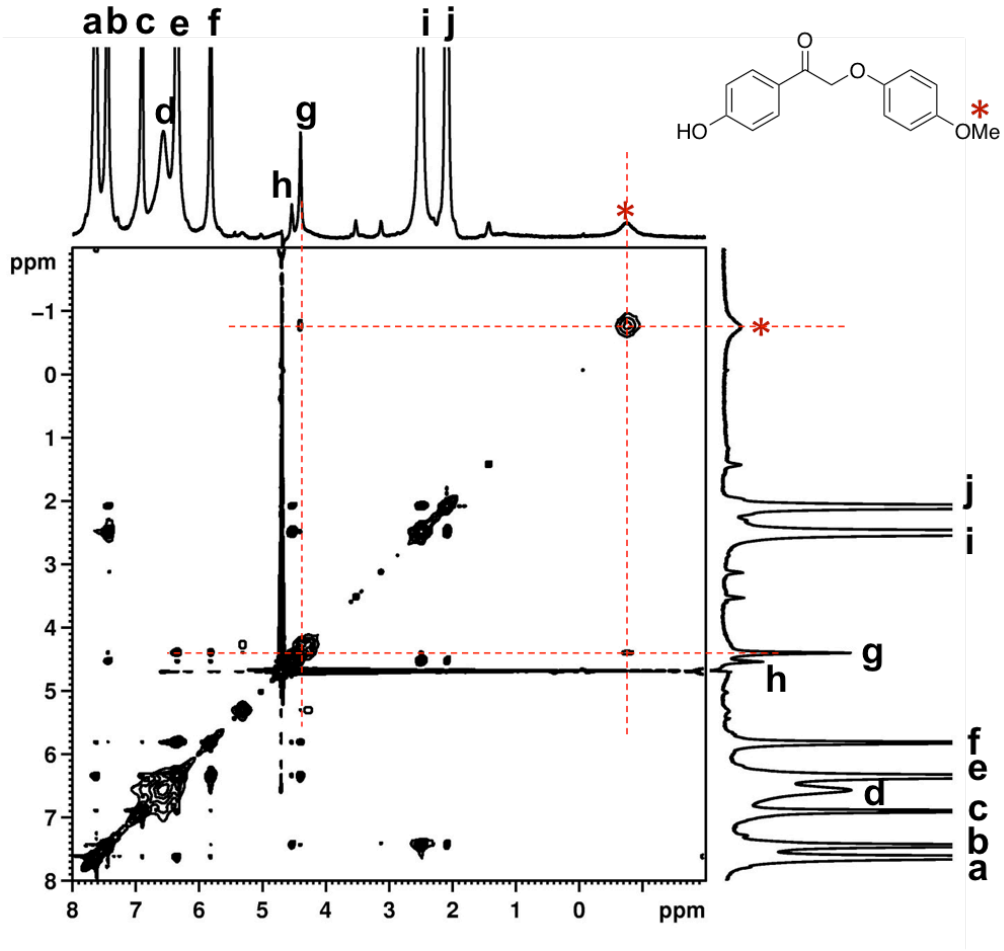


Figure S19. 2D-NOESY spectrum of **3f**@$(OA)_2$.

7. LC-DAD-MS and UHPLC-HR-MSn for pHP Phenyl Ethers 3c and 3f

7.1 Sample Preparation and Irradiation Conditions

Host-guest complexes **3c**@OA_2 and **3f**@OA_2 were prepared in borate buffer ($Na_2B_4O_7$, 10 mM, pH = 8.7) using 100 μM of guest and 200 μM of OA. Air equilibrated and N_2 purged solutions (gas bubbling for 5 min) were irradiated for different times and the decrease of trigger and formation of products followed by LC-DAD-MS. The irradiations were performed using a high-pressure xenon lamp in conjunction with a water filter to prevent heating of the sample solution and a Pyrex filter to remove UV radiation below 300 nm.

7.2 Instrumentation and Analysis Conditions

The LC-DAD-MS traces were obtained using an Agilent Technologies 1200 Series LC, equipped with a diode array detector, coupled to a Bruker Daltonics HCT *ultra* mass spectrometer. The MS analyses were performed using the following experimental conditions: ionization mode, negative polarity; capillary voltage, 4.0 kV; capillary exit voltage, -300 V; skimmer voltage, -15 V; drying gas, 320 ºC at 8 L min^{-1}; nebulizer gas pressure, 45 psi.

Depending on the sample and trigger, different columns and mobile phase gradient conditions were used. For analytical separation of OA, triggers and products, a mobile phase comprising water (A) and CH_3CN (B), both containing 0.1 % of formic acid, and ethyl acetate (C) was used. The gradient started with 52 % of A, 38 % of B and 10 % of C. The mobile phase composition was changed to 2 % of A, 73 % of B and 25 % of C in 5 min and kept at this composition for an additional 7 min. Finally, the system was allowed to return to the initial mobile phase composition (52 % of A, 38 % of B and 10 % of C) in 1 min and then stabilized for additional 5 min before the next run.

When better separation of photoproducts was necessary, as was the case for products of compound **3c**, a gradient with A and B, both containing 0.1 % of formic acid was used, followed by a cleaning step to remove OA, using a mixture of A, B, and C. In this case the gradient started with 85 % of A and 15 % of B. The mobile phase composition was changed to 10 % of A, 90 % of B in 5 min and then changed to 100 % of B in additional 6 min. The compositions were kept for 3 min in the case of **3f** and for 5 min in the case of **3c**. Then the column was washed with 2 % of A, 73 % of B and 25 % of C for 3 min to remove OA. Finally, the system was allowed to return to the initial mobile phase composition in 1 min and then stabilized for additional 5 min before the next run.

Three different columns were used: a) an Agilent PLRP-S LC column with 15.0 cm length, 2.1 mm internal diameter and 5 μm particle diameter; a b) silica based Grace RP-18, with 10.0 cm length, 2.1 mm internal diameter and 3 μm particle diameter, and c) an Agilent RP-18 with 15.0 cm length, 4.6 mm internal diameter and 5 μm particle diameter. The flow was 0.35 mL/min when the former two were used and 1.0 mL/min when the last one was used. Column a) was mainly used

for analysis of OA samples, column b) when better separation of products was required and column c) for LC-DAD operation (no MS). All columns were stabilized at 25 °C.

The non-irradiated and irradiated solutions were directly injected into the LC-DAD-MS system without further processing. In the analysis of samples containing borate buffer the mobile phase was sent to waste during the first 2 min to prevent contamination of the ion source with this non-volatile salt.

The UHPLC-HR-MSn studies were performed using a Thermo Scientific *ultimate* 3000 coupled to an Orbitrap Elite mass spectrometer. The HR-MSn analyses were achieved using the following experimental conditions: ionization mode, negative polarity; heater temperature, 300 ºC; capillary temperature, 350 ºC; spray voltage, 3.7 kV; S-Lenses RF level 68%. Fragmentation spectra of triggers and products were obtained by running the system in data dependent mode. A Thermo Accucore RP-18 column with 10.0 cm length, 2.1 mm internal diameter and 2.6 μm particle diameter was utilized. A mobile phase comprising water (A) and CH_3CN (B), both containing 0.1 % of formic acid, was used. The gradient started with 100 % of A. The mobile phase composition was changed to 30 % of B in 15 min and then raised to 100% of B in 16 min. This mobile phase composition (100 of % B) was kept for 4 min. Finally, the system was allowed to return to the initial mobile phase composition in 1 min and then stabilized for additional 4 min before the next run.

7.3 Identification and Quantification Studies on Non-irradiated and Irradiated Samples by LC-DAD-MS

The identification of products was achieved by injecting authentic standards and comparing the retentions times, m/z values and fragmentation patterns of these standards with the observed formed compounds. Photoproducts of **3c** and **3f** were monitored by LC-DAD with UV analysis at 280, 320, 350, 380 nm and by LC-MS/UHPLC-HRMSn under negative polarity. Quantitative analyses of triggers and photo-products were performed using calibrations curves prepared from DAD traces obtained at 280 nm.

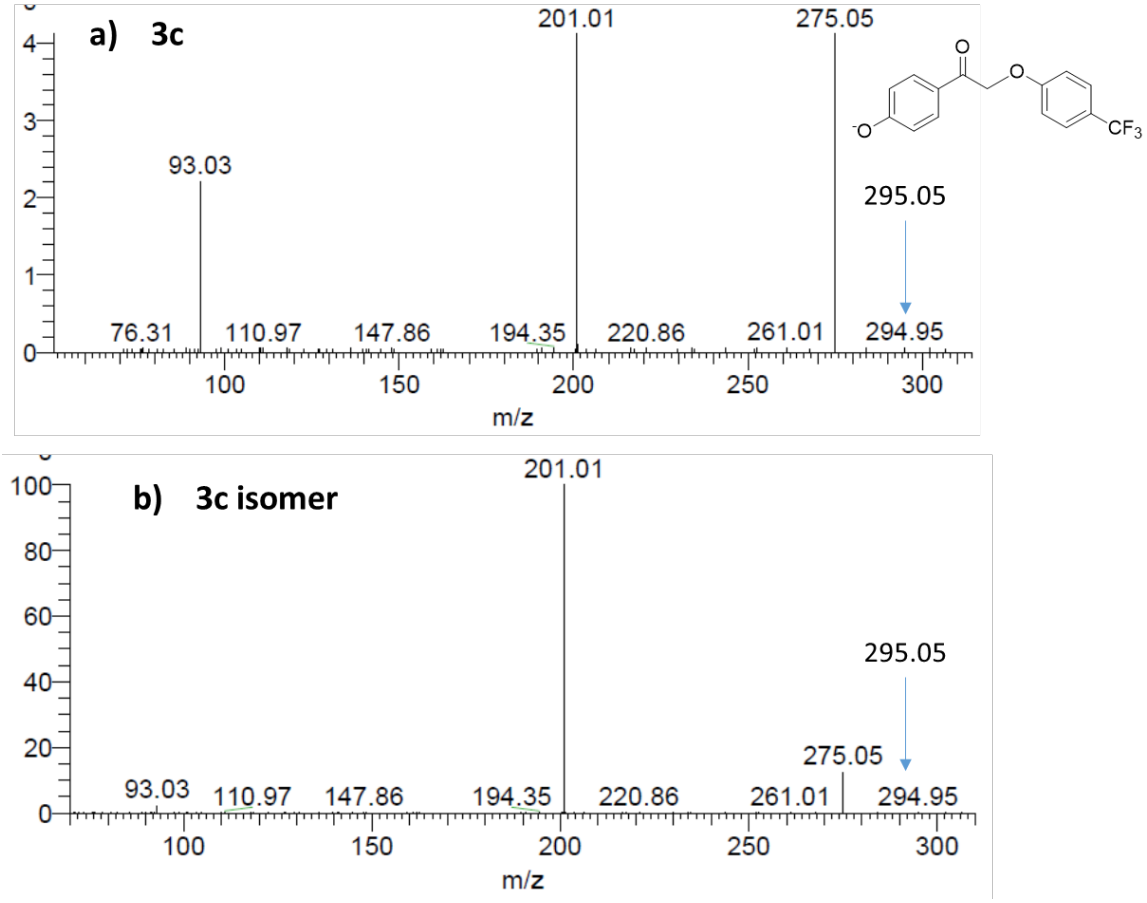


Figure S20. Fragmentation (CID) of compound **3c** (a), and that of the corresponding isomer (b). The arrow indicates the fragmented peak.

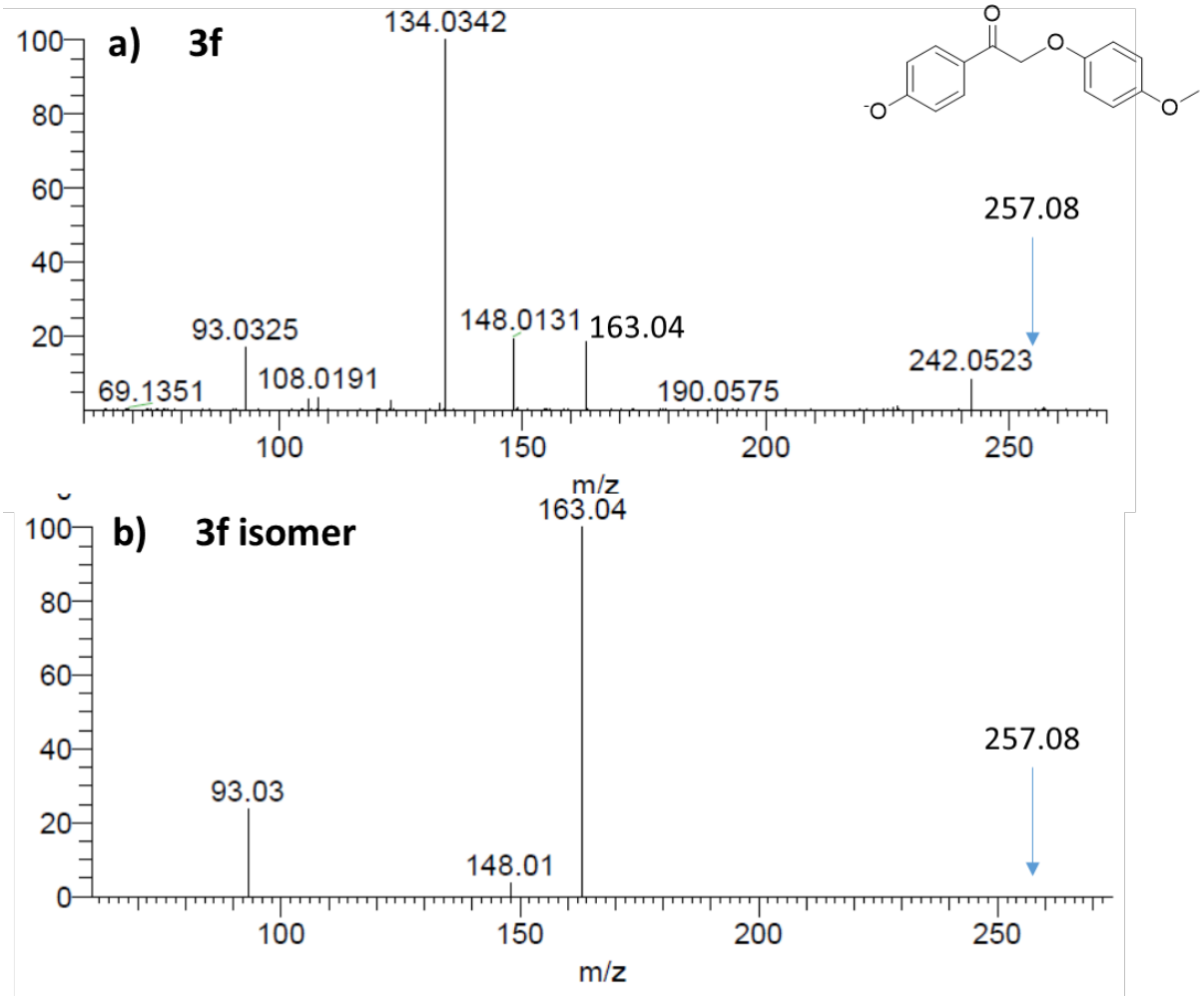


Figure S21. Fragmentation (CID) of compound **3f** (a), and that of the correspondent isomer (b). The arrow indicates the fragmented peak.

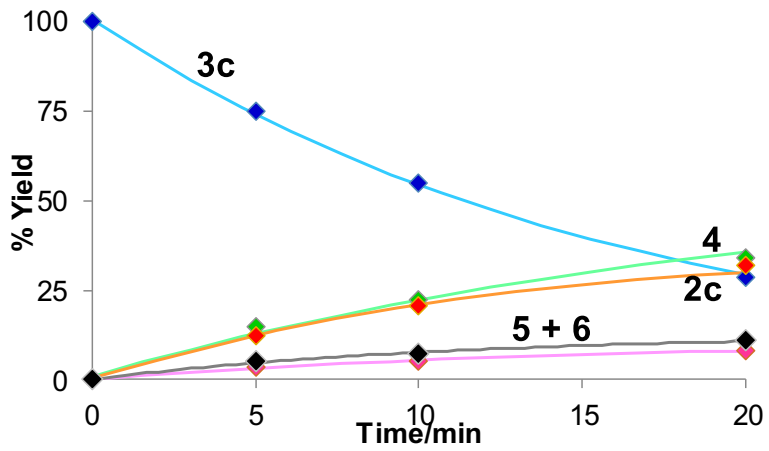


Figure S22. Reaction progress curves for the photolysis (λ > 300 nm) of **3c** encapsulated in OA (**3c**@$(OA)_2$). Disappearance of **3c** (blue), appearance of 4-methoxyphenol, **2c** (red), along with *p*-hydroxyphenylacetic acid, **4** (green), and trace amounts of 4-hydroxyacetophenone, **5** (black) and 2,4'-dihydroxyacetophenone, **6** (cyan) from the cage portion of **3c**. Solutions of complexes were prepared in aqueous borate buffer (pH = 8.7) at 2:1 stoichiometry (50 μM OA:100 μM of **3c**).

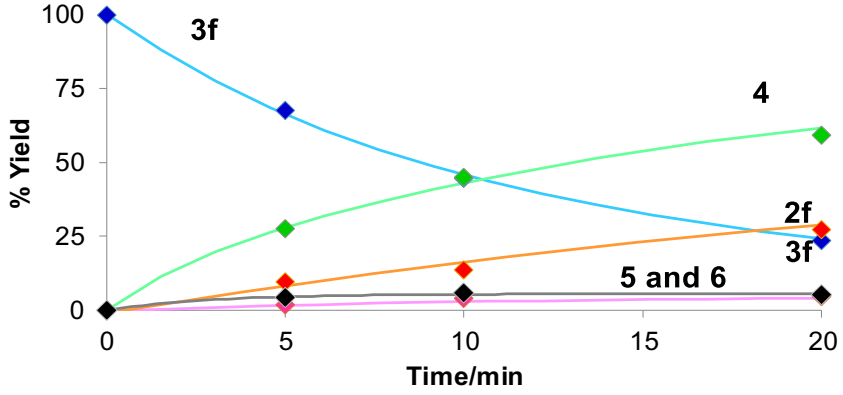


Figure S23. Reaction progress curves for the photolysis (λ > 300 nm) of **3f** encapsulated in OA (**3f**@$(OA)_2$). Disappearance of **3f** (blue), appearance of 4-methoxyphenol (**2f**, red), along with *p*-hydroxyphenylacetic acid (**4**, green) and trace amounts of 4-hydroxyacetophenone, **5** (black) and 2,4'-dihydroxyacetophenone, **6** (cyan) from the cage portion of **3f**. Solutions of complexes were prepared in aqueous borate buffer (pH = 8.7) at 2:1 stoichiometry (50 μM OA:100 μM of **3f**).

7.4 Effect of Oxygen on the Photochemistry of pHP Phenyl Ethers 3c and 3f in Acetonitrile and Mixtures Acetonitrile-Water of 20%-80%

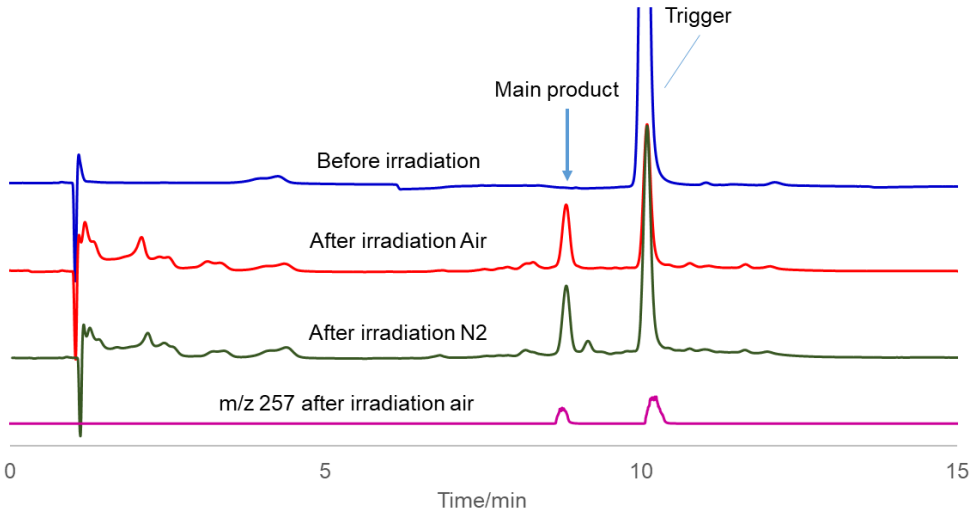


Figure S24. LC-DAD-MS profiles obtained after photolysis of **3f** in dry air equilibrated and N_2 purged CH_3CN.

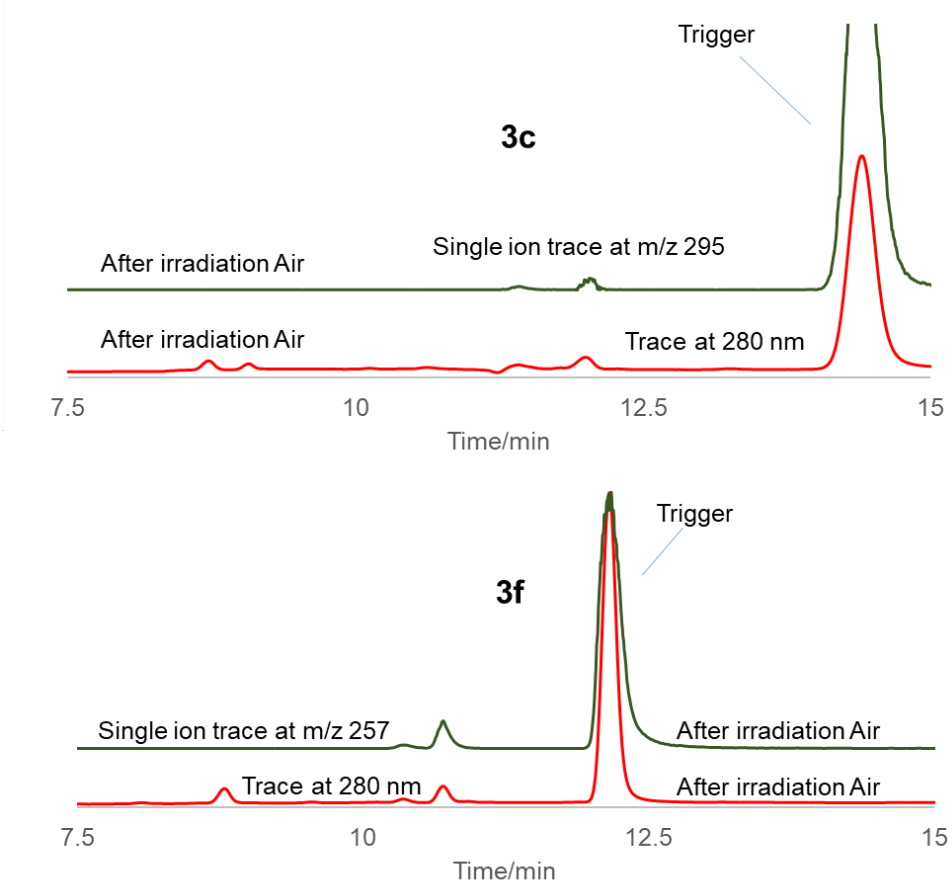


Figure S25. LC-DAD-MS profiles obtained after photolysis of **3c** and **3f** in air equilibrated water:CH_3CN mixture (80:20) showing the formation of rearrangement products.

8. Computational Studies

Compound **20** was optimized on the singlet and triplet state using uB3LYP/6-31+G(d,p) on G09 software.[6-10] The singlet energy was corrected for spin contamination using the following equation.

$$E_{singlet} = \frac{2E_{<S_z>=0} - < S^2 > E_{<S_z>=1}}{2 - < S^2 >}$$

Where E_{singlet} is the spin-corrected singlet energy, $E_{<S_z>=0}$ is the unrestricted singlet state energy, $< S^2 >$ is the expectation value of the total-spin operator for the broken-symmetry singlet calculation, and $E_{<S_z>=1}$ is the energy of the triplet state at the singlet geometry.

Compound **20** (optimized singlet state geometry)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.087836	-1.223191	0.059299
2	6	0	-1.460755	-1.226204	0.068643
3	6	0	-2.211401	0.020827	0.004404
4	6	0	-1.440155	1.253116	-0.069627
5	6	0	-0.064930	1.227307	-0.071772
6	1	0	0.480087	-2.146673	0.099487
7	1	0	-2.032911	-2.147076	0.122793
8	1	0	-1.995832	2.183710	-0.125315
9	1	0	0.477696	2.163930	-0.139512
10	6	0	0.640413	-0.004264	-0.004283
11	6	0	2.140063	-0.098150	-0.017113
12	6	0	2.934053	1.091240	0.141959
13	8	0	2.696541	-1.203398	-0.144098
14	1	0	2.519072	2.083097	0.273048
15	1	0	4.011942	0.973393	0.149181
16	8	0	-3.466137	0.034088	0.013005

Singlet Energy: -458.84345547 Hartrees

Spin-corrected Energy: -458.843453521 Hartrees

Compound **20** (optimized triplet state geometry)

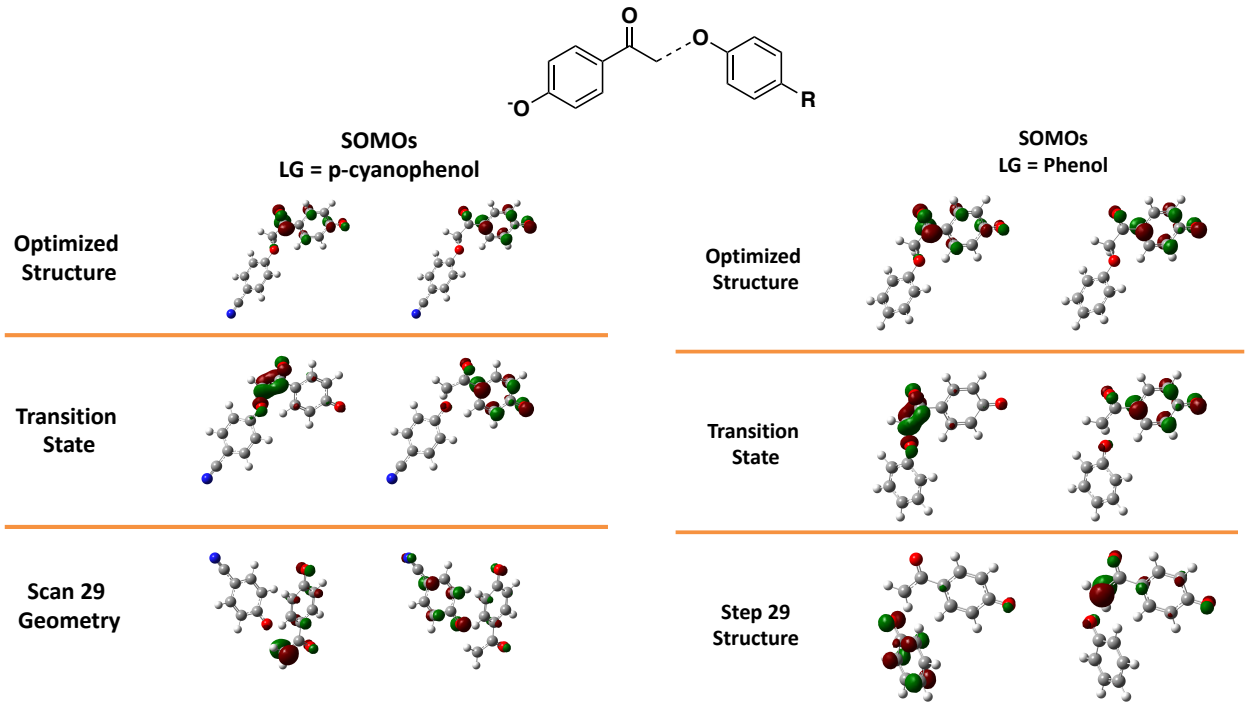
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.091350	-1.224794	0.060773
2	6	0	1.464705	-1.224184	0.072363
3	6	0	2.212238	0.022290	0.006383
4	6	0	1.437993	1.253142	-0.076142
5	6	0	0.062627	1.224767	-0.080604
6	1	0	-0.470972	-2.151232	0.104407
7	1	0	2.037826	-2.144071	0.130360
8	1	0	1.992146	2.184348	-0.137279
9	1	0	-0.484883	2.158461	-0.156161

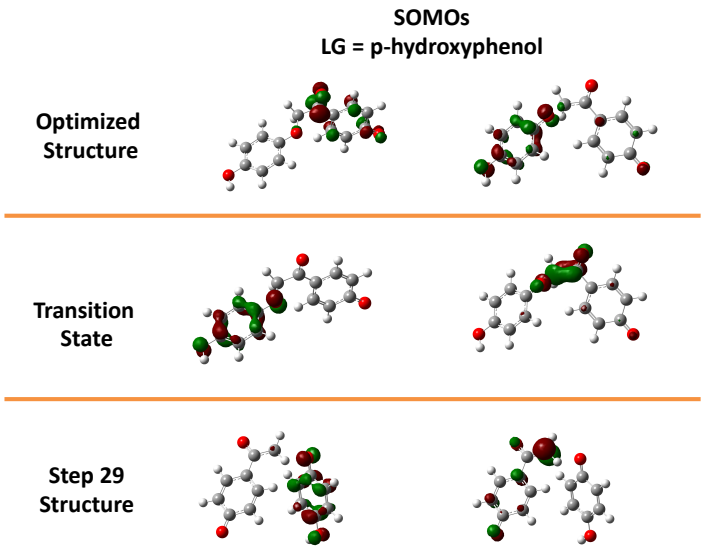
10	6	0	-0.639284	-0.007330	-0.005257
11	6	0	-2.132181	-0.084714	-0.013834
12	6	0	-2.954559	1.078344	0.150062
13	8	0	-2.685053	-1.202407	-0.151308
14	1	0	-2.563627	2.065383	0.366211
15	1	0	-4.028209	0.941744	0.093147
16	8	0	3.467601	0.042437	0.015914

Triplet Energy: -458.84387534 Hartrees

B. Relaxed scans of C-O bond

A relaxed scan on the bond length between the deprotonated pHP and phenolic leaving groups (as shown below) was done using B3LYP(6-31+G(d,p)) with SMD water solvent model using Gaussian 09.





p-hydroxyphenol leaving group

Geometry 1:
Energy: -841.11284323 Hartrees

C	4.49765200	-1.31436700	-0.06382400
C	3.14894900	-1.67174200	-0.44695600
C	2.12260500	-0.75371000	-0.44282300
C	2.34891800	0.62102600	-0.07895800
C	3.68443000	0.97890500	0.32777400
C	4.70825000	0.05601800	0.32988100
H	2.96458500	-2.70477400	-0.73139300
H	1.12412500	-1.07727100	-0.71688100
H	3.86237300	2.00610300	0.62452200
H	5.71232800	0.34412500	0.63234900
O	5.44961000	-2.18313800	-0.06373200
C	-0.07292800	1.30156300	-0.57989900
H	-0.58022600	2.22908500	-0.86680800
H	-0.07612600	0.61183000	-1.43405900
O	1.55861600	2.83466500	0.32507500
C	1.30890800	1.63315100	-0.10209200
O	-0.83374200	0.67070400	0.50623900
C	-2.12109100	0.26982200	0.25675300
C	-2.77870700	-0.38857400	1.30833200
C	-2.80527000	0.47557300	-0.95046000

C	-4.09144200	-0.83378300	1.16092900
H	-2.24884000	-0.54761800	2.24249900
C	-4.12308300	0.02501000	-1.09669300
H	-2.33328700	0.98270000	-1.78292800
C	-4.76914900	-0.62881200	-0.04789600
H	-4.65110400	0.18399100	-2.03197200
H	-4.58449900	-1.34126100	1.98660100
O	-6.06642600	-1.04890800	-0.25529000
H	-6.40203300	-1.49396700	0.53533400

Geom 2:
Energy: -841.11202221 Hartrees

C	4.50547900	-1.31738200	-0.05908500
C	3.15755100	-1.67601100	-0.44422900
C	2.13216100	-0.75670000	-0.44601200
C	2.35870400	0.61775000	-0.08782400
C	3.69134300	0.97696700	0.32080900
C	4.71573500	0.05458800	0.32970200
H	2.97334400	-2.71006300	-0.72465600
H	1.13410300	-1.08089200	-0.72080300
H	3.86809300	2.00543000	0.61383700
H	5.71897400	0.34373400	0.63357700
O	5.45601200	-2.18554000	-0.05300400
C	-0.05442300	1.30840400	-0.59973500
H	-0.57002600	2.22767300	-0.89056500
H	-0.07471200	0.59046000	-1.42664800
O	1.56849600	2.83094600	0.32364500
C	1.31798400	1.63341900	-0.11675600
O	-0.85132300	0.68395500	0.53202600
C	-2.13225100	0.27760200	0.27125900
C	-2.80082500	-0.37748600	1.31952600
C	-2.80796300	0.47306500	-0.94353400
C	-4.11123000	-0.82683400	1.16232800
H	-2.28037000	-0.53040500	2.26006500
C	-4.12303200	0.01795400	-1.09988300
H	-2.33068500	0.97668300	-1.77511200
C	-4.77811200	-0.63109400	-0.05381300
H	-4.64211600	0.17011200	-2.04138100
H	-4.61060800	-1.33080100	1.98648800
O	-6.07287400	-1.05581000	-0.27146400
H	-6.41522100	-1.49578700	0.51905600

Geom 3:
Energy: -841.11025175 Hartrees

C	4.50280600	-1.32788000	-0.05856200
C	3.15349800	-1.68133600	-0.44449500
C	2.13335400	-0.75602200	-0.44967000
C	2.36702100	0.61623200	-0.09539100
C	3.69863000	0.97064500	0.31324900
C	4.71961300	0.04444300	0.32644800
H	2.96456000	-2.71517300	-0.72211900
H	1.13388500	-1.07570800	-0.72452000
H	3.87892500	1.99933100	0.60332400
H	5.72377100	0.32979500	0.63041900
O	5.44785300	-2.19930900	-0.04908300
C	-0.03451100	1.32821900	-0.61374900
H	-0.55773100	2.24251900	-0.90007100
H	-0.07537500	0.58915800	-1.41817000
O	1.58710600	2.83144000	0.32908000
C	1.32940600	1.64070700	-0.12732400
O	-0.86755400	0.70457400	0.55984600
C	-2.14013300	0.28908200	0.28789800
C	-2.81437100	-0.37768400	1.32681900
C	-2.81144000	0.48543100	-0.93052000
C	-4.12105800	-0.83431800	1.15799300
H	-2.30036800	-0.53334900	2.27053800
C	-4.12217200	0.02235700	-1.09897200
H	-2.33285300	0.99749900	-1.75622000
C	-4.78095200	-0.63637100	-0.06135300
H	-4.63538500	0.17650300	-2.04345600
H	-4.62274400	-1.34619700	1.97600400
O	-6.07208300	-1.06826000	-0.29058000
H	-6.41740600	-1.51296600	0.49594400

Geom 4:
Energy: -841.10806812 Hartrees

C	4.48738700	-1.34770600	-0.06349900
C	3.13324900	-1.68918000	-0.44432400
C	2.12354600	-0.75229500	-0.44949700

C	2.37345000	0.61630200	-0.10090300
C	3.70730500	0.95941200	0.30147600
C	4.71999200	0.02418600	0.31559400
H	2.93295300	-2.72191300	-0.71757600
H	1.11978300	-1.06187900	-0.72015500
H	3.89769800	1.98769300	0.58657500
H	5.72786200	0.30057600	0.61498400
O	5.42208500	-2.22714100	-0.05366900
C	-0.01286800	1.36307400	-0.62069800
H	-0.54102000	2.27608500	-0.89600600
H	-0.07854100	0.60804800	-1.40597400
O	1.61640300	2.83639600	0.34169800
C	1.34365000	1.65564300	-0.13221800
O	-0.88371800	0.73794900	0.59190700
C	-2.14491500	0.30729200	0.30783400
C	-2.81773000	-0.38957500	1.32962800
C	-2.81646900	0.51659300	-0.90986900
C	-4.11838600	-0.85861400	1.14644600
H	-2.30667900	-0.55772000	2.27291200
C	-4.12018300	0.03996100	-1.09346300
H	-2.34199700	1.05163700	-1.72341700
C	-4.77571600	-0.64605400	-0.07155700
H	-4.63112800	0.20565800	-2.03733200
H	-4.61707800	-1.39220100	1.95249500
O	-6.06115800	-1.08959500	-0.31480700
H	-6.40460500	-1.55108300	0.46278200

Geom 5:
Energy: -841.10590293 Hartrees

C	4.43093700	-1.39531400	-0.08241500
C	3.06395700	-1.70242400	-0.44805300
C	2.08059400	-0.73779800	-0.44490900
C	2.37181600	0.62191600	-0.10296200
C	3.71565700	0.93185100	0.28378800
C	4.70446600	-0.02845900	0.29044700
H	2.83353900	-2.73007500	-0.71616600
H	1.06571100	-1.01997900	-0.70369900
H	3.93494500	1.95584600	0.56365500
H	5.72247300	0.22164200	0.57787200
O	5.34084300	-2.29690200	-0.08040200
C	0.01190900	1.44102100	-0.61185600
H	-0.51076400	2.36205700	-0.86418500

H	-0.09288700	0.67950700	-1.38455600
O	1.67461000	2.85642400	0.36594400
C	1.36607700	1.69264600	-0.12620700
O	-0.89846100	0.81374800	0.63781500
C	-2.13926700	0.34853800	0.33761700
C	-2.78344200	-0.43351500	1.31727600
C	-2.82890200	0.60510200	-0.86269700
C	-4.07001800	-0.93302300	1.11317700
H	-2.26132400	-0.64156700	2.24656200
C	-4.11635100	0.09556000	-1.06920300
H	-2.37900600	1.20665800	-1.64339400
C	-4.74229300	-0.67121200	-0.08664500
H	-4.63893800	0.29971700	-1.99919200
H	-4.54553300	-1.52993500	1.88840500
O	-6.01469400	-1.14257500	-0.34976700
H	-6.33742600	-1.65877300	0.40183200

Geom 6:
Energy: -841.10424111 Hartrees

C	4.15325700	-1.57130200	-0.12480800
C	2.74181400	-1.74717400	-0.39848200
C	1.86614100	-0.68395400	-0.37866200
C	2.31753200	0.64588900	-0.11063300
C	3.70442100	0.82886800	0.18461900
C	4.58922200	-0.22738100	0.17473300
H	2.39173100	-2.75406400	-0.60888400
H	0.81261500	-0.86388300	-0.56314000
H	4.04374500	1.83355900	0.40922000
H	5.64327400	-0.07607100	0.39189800
O	4.96324000	-2.55992500	-0.13676800
C	0.04645600	1.69516100	-0.56275700
H	-0.41356000	2.65567000	-0.78124100
H	-0.16797300	0.93896500	-1.31634600
O	1.86265800	2.94229700	0.35865100
C	1.42059400	1.81771200	-0.11821400
O	-0.91635400	1.12941300	0.74345800
C	-2.08338500	0.52433700	0.41497700
C	-2.56175300	-0.50040400	1.25658200
C	-2.86510400	0.87552200	-0.70477100
C	-3.77842700	-1.13723700	1.00350600
H	-1.96891800	-0.78700000	2.12036800
C	-4.07535700	0.22581400	-0.96767600

H	-2.53954500	1.66631100	-1.37180500
C	-4.53821500	-0.77866300	-0.11567800
H	-4.66849300	0.50466200	-1.83390200
H	-4.12838200	-1.91916700	1.67403400
O	-5.74396600	-1.37996700	-0.42426300
H	-5.95229300	-2.05665200	0.23475100

Geom 7:
Energy: -841.1032706 Hartrees

C	4.04489000	-1.62305800	-0.13275200
C	2.61933900	-1.75700100	-0.35610600
C	1.78364400	-0.66207700	-0.33977200
C	2.29134600	0.65461500	-0.12438000
C	3.69041300	0.79871900	0.12010500
C	4.53841300	-0.28677600	0.11281400
H	2.22836700	-2.75640900	-0.52549200
H	0.71856800	-0.80670100	-0.48475500
H	4.06966400	1.79749600	0.30459200
H	5.60366800	-0.16758700	0.29090900
O	4.81805700	-2.63750800	-0.14179100
C	0.06054200	1.78423600	-0.56345400
H	-0.38481500	2.75220700	-0.77331000
H	-0.20540200	1.01537000	-1.28538100
O	1.92204500	2.96574200	0.33799700
C	1.43205500	1.86186500	-0.13332500
O	-0.94231900	1.26033300	0.79574400
C	-2.06806100	0.59301700	0.46066900
C	-2.40513500	-0.58464400	1.15974400
C	-2.95094200	1.02998600	-0.55105800
C	-3.58361800	-1.28191100	0.88203200
H	-1.73385200	-0.94180700	1.93551800
C	-4.12044100	0.32319000	-0.84316600
H	-2.72680000	1.93615600	-1.10508300
C	-4.44355200	-0.83159000	-0.12559900
H	-4.79221600	0.67056300	-1.62304300
H	-3.82570200	-2.18131500	1.44424200
O	-5.61729600	-1.48447900	-0.45252400
H	-5.72873600	-2.26211100	0.11189500

Geom 8:

Energy: -841.10282543 Hartrees

C	3.97335900	-1.65378600	-0.12559500
C	2.53815200	-1.76180100	-0.29974500
C	1.72957600	-0.64673500	-0.29177700
C	2.27536500	0.66094400	-0.13347700
C	3.68221700	0.78167400	0.06427000
C	4.50577400	-0.32198500	0.06393900
H	2.11996300	-2.75655000	-0.42507100
H	0.65693900	-0.76792100	-0.39755000
H	4.08829900	1.77685300	0.20752700
H	5.57856900	-0.22347700	0.20457900
O	4.72212900	-2.68356600	-0.12853800
C	0.07610200	1.83750200	-0.58367400
H	-0.36831900	2.80543200	-0.79099900
H	-0.22074800	1.05155500	-1.27261300
O	1.95859500	2.98209600	0.30873500
C	1.43987000	1.89132400	-0.15329200
O	-0.96749200	1.34905100	0.82320300
C	-2.06216400	0.64028400	0.48909200
C	-2.29269800	-0.62318000	1.07571600
C	-3.02352000	1.11530600	-0.43277800
C	-3.44109600	-1.36370900	0.78255500
H	-1.56221700	-1.01239800	1.77953800
C	-4.16294500	0.36919600	-0.74151100
H	-2.87746800	2.08503900	-0.89953900
C	-4.37828300	-0.87062200	-0.13174800
H	-4.89500200	0.74779000	-1.44942700
H	-3.60065700	-2.32821600	1.26007100
O	-5.52767600	-1.56090100	-0.46879200
H	-5.56205600	-2.39800600	0.01477400

Geom 9:
Energy: -841.10292376 Hartrees

C	3.93066600	-1.67570800	-0.11941500
C	2.49034500	-1.76463400	-0.26436700
C	1.70070000	-0.63623700	-0.26242700
C	2.27135600	0.66299300	-0.13758600
C	3.68186400	0.76677800	0.03187000
C	4.48862200	-0.34874500	0.03581300
H	2.05478700	-2.75479800	-0.36324700

H	0.62425400	-0.73980100	-0.34593800
H	4.10531300	1.75806400	0.15041700
H	5.56534200	-0.26555700	0.15362100
O	4.66250100	-2.71529500	-0.11828600
C	0.09883200	1.87364900	-0.60683800
H	-0.34879800	2.84134600	-0.80380700
H	-0.21784800	1.07749100	-1.27314900
O	1.98648800	2.98731700	0.30186300
C	1.45184400	1.90948600	-0.16283100
O	-0.98762200	1.39948800	0.83750000
C	-2.06129600	0.66880600	0.50340000
C	-2.24853600	-0.62249400	1.04814400
C	-3.05242200	1.14370000	-0.38966300
C	-3.37933500	-1.38601800	0.74574800
H	-1.49783600	-1.01411700	1.72916100
C	-4.17486200	0.37641500	-0.70655700
H	-2.93891100	2.13228000	-0.82558700
C	-4.34493500	-0.88958800	-0.13666700
H	-4.92882200	0.75693500	-1.39018500
H	-3.50391400	-2.37062900	1.19176000
O	-5.47964000	-1.60131700	-0.48019600
H	-5.48443100	-2.45317400	-0.02184000

Geom 10:
Energy: -841.10339413 Hartrees

C	3.86687900	-1.71078600	-0.11624700
C	2.42242800	-1.76805800	-0.23905100
C	1.66047400	-0.62095400	-0.24156200
C	2.26438400	0.66415200	-0.14040200
C	3.67823000	0.73848400	0.00660900
C	4.45910700	-0.39487200	0.01285800
H	1.96257100	-2.74888700	-0.31818600
H	0.58069500	-0.69828700	-0.30886800
H	4.12626000	1.72107200	0.10635300
H	5.53914700	-0.33608500	0.11280700
O	4.57381700	-2.76565900	-0.11235300
C	0.13038700	1.92673200	-0.63113700
H	-0.31210600	2.89923000	-0.81140600
H	-0.20888400	1.12922700	-1.28305200
O	2.02630700	2.99018700	0.31030900
C	1.47136900	1.93185500	-0.16619300
O	-1.00559800	1.46382400	0.84396600
C	-2.05496400	0.70717600	0.51111000

C	-2.21683600	-0.58941700	1.05676500
C	-3.05445800	1.15432000	-0.39004100
C	-3.32730200	-1.37994000	0.74930300
H	-1.46203700	-0.96219200	1.74390600
C	-4.15673100	0.36060100	-0.71075000
H	-2.96012500	2.14399100	-0.82844200
C	-4.30003100	-0.90824800	-0.13900000
H	-4.91587000	0.72149300	-1.39939500
H	-3.43114600	-2.36651800	1.19640400
O	-5.41599900	-1.64738200	-0.48681700
H	-5.40432800	-2.49707100	-0.02451600

Geom 11:
Energy: -841.10413741 Hartrees

C	3.77290700	-1.75984200	-0.11344700
C	2.32623200	-1.77077200	-0.22649100
C	1.60313200	-0.59898500	-0.23470300
C	2.25039200	0.66492000	-0.14540500
C	3.66629000	0.69515500	-0.01004300
C	4.40992400	-0.46260200	-0.00072800
H	1.83382700	-2.73649200	-0.29370100
H	0.52099500	-0.64013500	-0.29492700
H	4.14699300	1.66331200	0.07853400
H	5.49206400	-0.43894800	0.08991100
O	4.44458800	-2.83614100	-0.10457900
C	0.17016500	1.99954700	-0.65939900
H	-0.25737900	2.98166900	-0.81902800
H	-0.19680500	1.20857600	-1.30285700
O	2.07912200	2.99172100	0.32525100
C	1.49733100	1.95987300	-0.16897000
O	-1.02183100	1.55039800	0.84141300
C	-2.04117700	0.75986700	0.51394100
C	-2.17742800	-0.53228200	1.08215900
C	-3.04218300	1.16005700	-0.41047000
C	-3.26090900	-1.35859200	0.77438100
H	-1.42349600	-0.87149200	1.78744800
C	-4.11748400	0.33064700	-0.73019700
H	-2.96718500	2.14288000	-0.86784700
C	-4.23386200	-0.93112200	-0.13608900
H	-4.87641300	0.65683500	-1.43624600
H	-3.34436400	-2.33903000	1.23890600
O	-5.32367700	-1.70768900	-0.48460100

H	-5.29383500	-2.54869200	-0.00730200

Geom 12:
Energy: -841.10506675 Hartrees

C	3.72318200	-1.78610500	-0.11079300
C	2.27748200	-1.77039800	-0.23745000
C	1.57657500	-0.58543500	-0.25154600
C	2.24598500	0.66552800	-0.15105100
C	3.66046500	0.67032500	-0.00385000
C	4.38310200	-0.50044500	0.00927000
H	1.76803700	-2.72678500	-0.31014600
H	0.49452900	-0.60652200	-0.32228700
H	4.15773600	1.62951800	0.09120700
H	5.46466400	-0.49669500	0.10898000
O	4.37502900	-2.87367100	-0.09744500
C	0.20381100	2.04148800	-0.69136900
H	-0.22115100	3.02696700	-0.83323700
H	-0.18101600	1.25178500	-1.32459400
O	2.10769100	2.99056000	0.33767000
C	1.51645700	1.97574300	-0.17359000
O	-1.03394900	1.59298300	0.83872000
C	-2.03575100	0.78677200	0.51646400
C	-2.15568900	-0.50639900	1.09158400
C	-3.04228700	1.16524600	-0.41440700
C	-3.22495200	-1.35027500	0.78496500
H	-1.39909800	-0.83027500	1.80121600
C	-4.10361300	0.31847100	-0.73157100
H	-2.97944200	2.14607200	-0.87795500
C	-4.20223300	-0.94220300	-0.13049200
H	-4.86575600	0.62851400	-1.44143900
H	-3.29529100	-2.32946500	1.25426300
O	-5.27879400	-1.73644000	-0.47738000
H	-5.23821900	-2.57445100	0.00449300

Geom 13:
Energy: -841.10615105 Hartrees

C	3.67881500	-1.80923300	-0.10991900
C	2.24007300	-1.76693400	-0.29504500

C	1.55910900	-0.57065000	-0.31564600
C	2.24129500	0.66750200	-0.15977800
C	3.64817000	0.64597700	0.04351100
C	4.35204600	-0.53621000	0.06225400
H	1.71860000	-2.71310100	-0.40616200
H	0.48074700	-0.57486200	-0.43055100
H	4.15576200	1.59507300	0.17811600
H	5.42861000	-0.55116000	0.20579800
O	4.31351100	-2.90670300	-0.09211200
C	0.23904000	2.08028000	-0.73309700
H	-0.18527600	3.06828000	-0.85563400
H	-0.16214900	1.29303500	-1.35778500
O	2.12852300	2.99150700	0.34730300
C	1.53496500	1.99052000	-0.18224000
O	-1.03618000	1.61888100	0.82884100
C	-2.02584500	0.80478000	0.51714200
C	-2.13632100	-0.48728700	1.10414800
C	-3.03774600	1.16648300	-0.41909200
C	-3.19695800	-1.34161500	0.80394500
H	-1.37643400	-0.79836100	1.81583200
C	-4.09093700	0.30922000	-0.72777100
H	-2.98121200	2.14348200	-0.89126400
C	-4.17826000	-0.94819300	-0.11536300
H	-4.85636600	0.60549000	-1.43987200
H	-3.25995000	-2.31784800	1.28022400
O	-5.24669300	-1.75252000	-0.45518600
H	-5.20029100	-2.58717800	0.03224900

Geom 14:
Energy: -841.10998290 Hartrees

C	4.32421500	-1.53918200	-0.01750700
C	3.06475600	-1.63637100	-0.71182300
C	2.17277300	-0.57904900	-0.77454400
C	2.43944800	0.67015500	-0.15640200
C	3.67309200	0.78252100	0.53256800
C	4.57757000	-0.26194200	0.60366400
H	2.82345200	-2.58127200	-1.19440300
H	1.24020700	-0.73044300	-1.31075600
H	3.90178900	1.72856900	1.01556200
H	5.51616700	-0.13894000	1.14076000
O	5.15764600	-2.51493000	0.04544900
C	0.29561600	1.74379900	-0.93637600

H	-0.29288400	2.64737600	-1.03282200
H	0.08146600	0.93247100	-1.61793600
O	1.78901000	2.89219300	0.44381200
C	1.51802600	1.82409800	-0.19604800
O	-1.04741200	0.97826200	0.51217800
C	-2.19204400	0.44863200	0.33612400
C	-2.85102900	-0.25517300	1.41811300
C	-2.88977800	0.51602600	-0.93225600
C	-4.08163400	-0.84209800	1.24409400
H	-2.33744200	-0.30719700	2.37252000
C	-4.11975000	-0.07208700	-1.09563400
H	-2.42173800	1.04829500	-1.75256100
C	-4.72681200	-0.75879600	-0.01433300
H	-4.64762500	-0.02371400	-2.04248500
H	-4.56461700	-1.36979600	2.06191800
O	-5.93092700	-1.31563800	-0.24855700
H	-6.27201100	-1.76765800	0.53929800

Geom 15:
Energy: -841.11243024 Hartrees

C	4.32675700	-1.54633100	-0.01794200
C	3.07843200	-1.62906200	-0.73435500
C	2.19184400	-0.56763800	-0.79689600
C	2.45337500	0.67177400	-0.15666200
C	3.67586300	0.76970900	0.55457300
C	4.57461500	-0.27901400	0.62625800
H	2.84235300	-2.56591000	-1.23482600
H	1.26837100	-0.70716800	-1.35158100
H	3.89950900	1.70803600	1.05463500
H	5.50444200	-0.16803900	1.18084800
O	5.15544900	-2.52532100	0.04453100
C	0.32541300	1.76386600	-0.95422200
H	-0.26667200	2.66613300	-1.03826600
H	0.10074800	0.95053200	-1.62968100
O	1.80827000	2.89223300	0.45194000
C	1.53907100	1.83018100	-0.19691400
O	-1.06356600	0.98090300	0.51551900
C	-2.20628600	0.44993200	0.34069000
C	-2.86509300	-0.25943500	1.41985000
C	-2.90515400	0.52086900	-0.92760700
C	-4.09505800	-0.84711100	1.24319300
H	-2.35183200	-0.31478600	2.37429500

C	-4.13430700	-0.06815000	-1.09364700
H	-2.43626700	1.05668900	-1.74530900
C	-4.74035900	-0.75965300	-0.01486700
H	-4.66218900	-0.01714300	-2.04039100
H	-4.57764500	-1.37874200	2.05874600
O	-5.94405700	-1.31740200	-0.25105500
H	-6.28425500	-1.77252700	0.53535100

Geom 16:
Energy: -841.11461604 Hartrees

C	4.32770400	-1.55516700	-0.02193300
C	3.08688200	-1.62383200	-0.75320100
C	2.20663700	-0.55749900	-0.81365800
C	2.46755500	0.67343500	-0.15642800
C	3.68250400	0.75732300	0.56995100
C	4.57478300	-0.29641400	0.63999900
H	2.85241300	-2.55366100	-1.26723800
H	1.28934000	-0.68554700	-1.38107500
H	3.90480800	1.68887600	1.08306600
H	5.49886800	-0.19699100	1.20616400
O	5.15091000	-2.53809200	0.03808000
C	0.35376800	1.78473200	-0.96443900
H	-0.24028400	2.68658800	-1.03651900
H	0.11692800	0.96977000	-1.63353600
O	1.83153900	2.89328400	0.46155200
C	1.56115900	1.83701600	-0.19491300
O	-1.08152000	0.98636700	0.52698400
C	-2.22141900	0.45287600	0.34963600
C	-2.87660100	-0.27402800	1.41990300
C	-2.92334900	0.53788400	-0.91675000
C	-4.10492200	-0.86342200	1.23686000
H	-2.36188200	-0.34097200	2.37286800
C	-4.15072100	-0.05298800	-1.08916500
H	-2.45627700	1.08622900	-1.72733500
C	-4.75263600	-0.76089300	-0.01878800
H	-4.68029200	0.00871100	-2.03436700
H	-4.58457200	-1.40800300	2.04563000
O	-5.95524600	-1.31948900	-0.26045600
H	-6.29259400	-1.78570400	0.52062100

Geom 17:
Energy: -841.11655503 Hartrees

C	4.36853300	-1.53867800	-0.03585500
C	3.13022800	-1.60967400	-0.77156300
C	2.24203000	-0.54993900	-0.82358100
C	2.49165600	0.67624900	-0.15268400
C	3.70441300	0.76264400	0.57754800
C	4.60462000	-0.28437300	0.63912400
H	2.90469600	-2.53603900	-1.29566900
H	1.32731300	-0.67925600	-1.39477400
H	3.91801500	1.69077100	1.10043600
H	5.52677800	-0.18354300	1.20809400
O	5.19855400	-2.51559500	0.01712500
C	0.37227100	1.77921300	-0.95660600
H	-0.23628800	2.67259700	-1.01049800
H	0.13441800	0.96378800	-1.62467600
O	1.83489500	2.88334300	0.48742700
C	1.57595000	1.83184700	-0.18024100
O	-1.09451600	0.92622800	0.54907800
C	-2.24288500	0.41652000	0.36342300
C	-2.89756400	-0.34949100	1.40703600
C	-2.95786200	0.56861600	-0.88984800
C	-4.13698900	-0.91143600	1.21196900
H	-2.37357200	-0.46762900	2.34996300
C	-4.19602200	0.00478100	-1.07444500
H	-2.49008500	1.14542300	-1.68008500
C	-4.79700600	-0.74138600	-0.02992300
H	-4.73507700	0.11669800	-2.00964900
H	-4.61656100	-1.48522200	2.00060700
O	-6.01144700	-1.26930700	-0.28248900
H	-6.34774900	-1.76428800	0.48100700

Geom 18:
Energy: -841.11827007 Hartrees

C	4.37236100	-1.54601600	-0.04165300
C	3.13956800	-1.60448000	-0.78806400
C	2.25693900	-0.54039800	-0.83709800
C	2.50710400	0.67832500	-0.15231200
C	3.71430900	0.75218300	0.58893000
C	4.60893100	-0.29927300	0.64774100
H	2.91448300	-2.52470500	-1.32296700

H	1.34667500	-0.65968700	-1.41741300
H	3.92756100	1.67430100	1.12245800
H	5.52695700	-0.20854200	1.22494600
O	5.19744800	-2.52656400	0.00817300
C	0.39941300	1.79804100	-0.96233800
H	-0.21114500	2.69064000	-1.00510600
H	0.15104100	0.98175300	-1.62544800
O	1.85771600	2.88403400	0.49909600
C	1.59794800	1.83828900	-0.17649300
O	-1.11248300	0.92620600	0.56395100
C	-2.25909500	0.41620300	0.37371500
C	-2.90896300	-0.37273700	1.40361600
C	-2.97878500	0.59078600	-0.87435200
C	-4.14759700	-0.93395900	1.20089300
H	-2.38207400	-0.50840000	2.34260400
C	-4.21594900	0.02740700	-1.06672400
H	-2.51372200	1.18431600	-1.65385300
C	-4.81177500	-0.74084900	-0.03539300
H	-4.75811300	0.15616600	-1.99798700
H	-4.62351100	-1.52459600	1.97931800
O	-6.02592400	-1.26680300	-0.29486600
H	-6.35866900	-1.77736600	0.45981300

Geom 19:
Energy: -841.11977473 Hartrees

C	4.37845100	-1.55210500	-0.04553200
C	3.15098900	-1.59957200	-0.80183200
C	2.27334400	-0.53166500	-0.84887000
C	2.52357200	0.68048400	-0.15197700
C	3.72546000	0.74340900	0.59928600
C	4.61510300	-0.31193500	0.65623000
H	2.92657700	-2.51447800	-1.34598500
H	1.36730900	-0.64219700	-1.43738600
H	3.93812800	1.66032800	1.14191800
H	5.52917600	-0.22998400	1.24089400
O	5.19908200	-2.53587800	0.00215400
C	0.42756600	1.81525800	-0.96966300
H	-0.18559100	2.70656800	-1.00193800
H	0.17135700	0.99894600	-1.62972300
O	1.87904600	2.88412200	0.51059800
C	1.61999800	1.84409700	-0.17340900
O	-1.12908900	0.92035400	0.57494200
C	-2.27531500	0.41248100	0.38122800

C	-2.92420200	-0.39053900	1.40119400
C	-2.99729500	0.60393200	-0.86336100
C	-4.16357700	-0.94825000	1.19278300
H	-2.39615700	-0.53917500	2.33760000
C	-4.23490700	0.04365100	-1.06166600
H	-2.53195100	1.20743300	-1.63511000
C	-4.82946700	-0.73805900	-0.03978900
H	-4.77840000	0.18485400	-1.99036900
H	-4.63881600	-1.54888300	1.96402300
O	-6.04449700	-1.25987800	-0.30461000
H	-6.37627900	-1.78029400	0.44366300

Geom 20:
Energy: -841.12108797 Hartrees

C	4.39055400	-1.55554700	-0.04790300
C	3.16787300	-1.59498800	-0.81271300
C	2.29349900	-0.52469300	-0.85849900
C	2.54250700	0.68232500	-0.15181500
C	3.73968200	0.73728600	0.60795400
C	4.62607600	-0.32046800	0.66371700
H	2.94494800	-2.50576700	-1.36427600
H	1.39129500	-0.62882500	-1.45396200
H	3.95093500	1.65015000	1.15790800
H	5.53662800	-0.24489300	1.25463500
O	5.20815700	-2.54135300	-0.00142800
C	0.45532400	1.82754000	-0.97603500
H	-0.16096500	2.71706800	-0.99948500
H	0.19312700	1.01077100	-1.63317700
O	1.89974500	2.88356800	0.51999100
C	1.64247500	1.84806100	-0.17104300
O	-1.14694500	0.90812300	0.58492400
C	-2.29401200	0.40497800	0.38767900
C	-2.94579400	-0.40598400	1.39978200
C	-3.01566800	0.61045600	-0.85514300
C	-4.18729200	-0.95710600	1.18613400
H	-2.41838000	-0.56551500	2.33478100
C	-4.25517400	0.05639000	-1.05889300
H	-2.54706000	1.21924700	-1.62084900
C	-4.85249100	-0.73267500	-0.04430100
H	-4.79813700	0.20793300	-1.98629800
H	-4.66476000	-1.56326000	1.95171400
O	-6.06967200	-1.24742900	-0.31397500

H	-6.40327200	-1.77362100	0.42938800

Geom 21:
Energy: -841.12223247 Hartrees

C	4.39874500	-1.56243800	-0.05107900
C	3.17946100	-1.59300200	-0.82202300
C	2.30998800	-0.51900900	-0.86650600
C	2.56101000	0.68350300	-0.15236600
C	3.75494500	0.72973300	0.61345800
C	4.63636700	-0.33185100	0.66814900
H	2.95568100	-2.50005000	-1.37928700
H	1.41050400	-0.61610500	-1.46718000
H	3.96721300	1.63906200	1.16883600
H	5.54445100	-0.26333900	1.26365200
O	5.21181700	-2.55150500	-0.00588000
C	0.48152700	1.84028800	-0.97848200
H	-0.13473600	2.73006700	-0.99577100
H	0.20976400	1.02155800	-1.62929400
O	1.92700000	2.88584700	0.52379000
C	1.66671300	1.85312600	-0.16993500
O	-1.16884600	0.90708000	0.60231800
C	-2.31448100	0.40452500	0.39858100
C	-2.96587800	-0.42176000	1.39874900
C	-3.03608300	0.62620400	-0.84174900
C	-4.20660200	-0.97140100	1.17666000
H	-2.43890900	-0.59359200	2.33184200
C	-4.27462800	0.07326300	-1.05412600
H	-2.56692300	1.24605800	-1.59828300
C	-4.87136000	-0.73066700	-0.05093100
H	-4.81726900	0.23672900	-1.97971000
H	-4.68390300	-1.58864100	1.93346800
O	-6.08787000	-1.24325100	-0.32847900
H	-6.42103200	-1.78018900	0.40731500

Geom 22:
Energy: -841.12322945 Hartrees

C	4.34857100	-1.59701500	-0.07973700
C	3.12437300	-1.59469400	-0.84383300
C	2.27913300	-0.50152400	-0.87512300

C	2.56166700	0.68989700	-0.15346000
C	3.76102500	0.70384200	0.60573000
C	4.61821800	-0.37753700	0.64779300
H	2.87808300	-2.49239500	-1.40667300
H	1.37472800	-0.57352200	-1.47189400
H	3.99689500	1.60416900	1.16624000
H	5.53089700	-0.33427600	1.23865300
O	5.13927100	-2.60381500	-0.04731900
C	0.49874200	1.89470200	-0.94984300
H	-0.10087000	2.79604800	-0.95236300
H	0.19184400	1.07859200	-1.58822800
O	1.98878600	2.90594500	0.53224400
C	1.69519400	1.87998100	-0.15792500
O	-1.18389300	0.95027400	0.66870000
C	-2.31671400	0.43048800	0.44056100
C	-2.91362900	-0.51912900	1.36242500
C	-3.07737400	0.75306300	-0.75362200
C	-4.13999600	-1.08821100	1.11097200
H	-2.35721200	-0.76771200	2.26053200
C	-4.30115400	0.17984300	-0.99578800
H	-2.64883100	1.46530500	-1.45071400
C	-4.84378700	-0.74581400	-0.06982900
H	-4.87273100	0.41847200	-1.88701600
H	-4.57615300	-1.79831800	1.80898100
O	-6.04890000	-1.27111200	-0.37316100
H	-6.34437600	-1.89405600	0.30885000

Geom 23:
Energy: -841.1237670 Hartrees

C	3.39197200	-2.03208000	-0.10538400
C	2.23425200	-1.67454800	-0.89338800
C	1.73844700	-0.38448700	-0.92792900
C	2.33600200	0.67319900	-0.18880900
C	3.47439400	0.33996100	0.59226800
C	3.98604700	-0.94181200	0.63904600
H	1.75205800	-2.46138000	-1.46918200
H	0.86307700	-0.19120200	-1.54052600
H	3.94586200	1.13328600	1.16535000
H	4.86050600	-1.16434700	1.24692700
O	3.86111100	-3.22933500	-0.06642500
C	0.69985000	2.41159500	-0.99474000
H	0.35430600	3.43770100	-0.97601300
H	0.18727300	1.71616400	-1.64441700

O	2.40791700	2.97047800	0.52410600
C	1.83997800	2.06232500	-0.18900400
O	-1.24371500	1.91233200	0.60854600
C	-2.13193400	1.01330700	0.42527000
C	-2.34734500	-0.05195400	1.39128200
C	-2.96966600	0.99662700	-0.76370000
C	-3.29611000	-1.02641600	1.18516300
H	-1.73008800	-0.05553200	2.28402200
C	-3.91566400	0.01958700	-0.95882400
H	-2.82531300	1.78602100	-1.49433000
C	-4.08739800	-1.00089200	0.01008000
H	-4.54237500	0.00592500	-1.84494500
H	-3.44552500	-1.81912500	1.91364100
O	-5.03237400	-1.93169000	-0.24561800
H	-5.08024600	-2.58826500	0.46661700

Geom 24:
Energy: -841.12511548 Hartrees

C	3.38455600	-2.03725500	-0.10238000
C	2.23565400	-1.67105500	-0.89694300
C	1.74803200	-0.37933100	-0.93011300
C	2.34690000	0.67122200	-0.18195500
C	3.47723500	0.32808700	0.60645300
C	3.98002600	-0.95573500	0.65111400
H	1.75360400	-2.45304200	-1.47924800
H	0.87864400	-0.17836800	-1.54848500
H	3.94907900	1.11612000	1.18632800
H	4.84860300	-1.18672200	1.26406300
O	3.84382900	-3.23031700	-0.06568700
C	0.73603700	2.42489800	-0.99162100
H	0.39883400	3.45378800	-0.96790600
H	0.21811300	1.73717800	-1.64497400
O	2.42299700	2.94986400	0.53365800
C	1.86146300	2.06068600	-0.18000900
O	-1.32668800	1.97921400	0.55857900
C	-2.17661600	1.05440400	0.39670000
C	-2.36361300	0.01123900	1.38913200
C	-3.00331000	0.98042900	-0.79515200
C	-3.27963400	-0.99775300	1.20410900
H	-1.75297200	0.05175100	2.28555200
C	-3.91621900	-0.03045500	-0.97058000
H	-2.87706400	1.75448000	-1.54537500

C	-4.06244600	-1.02930400	0.02395500
H	-4.53534200	-0.08780300	-1.86020200
H	-3.40900900	-1.77429000	1.95364300
O	-4.97459100	-1.99590400	-0.21330100
H	-5.00525900	-2.63641200	0.51436800

Geom 25:
Energy: -841.12585075 Hartrees

C	3.38285500	-2.04534800	-0.10483500
C	2.24572300	-1.66692700	-0.91063500
C	1.76745800	-0.37181800	-0.94233200
C	2.36492600	0.67054500	-0.18139900
C	3.48370500	0.31529500	0.61823100
C	3.97694600	-0.97210500	0.66173400
H	1.76534600	-2.44242900	-1.50287700
H	0.90713900	-0.16138700	-1.57014800
H	3.95402100	1.09692500	1.20791400
H	4.83659100	-1.21260600	1.28352200
O	3.83357000	-3.24148800	-0.06956300
C	0.77228000	2.43839200	-0.99553100
H	0.44040900	3.46911600	-0.96803400
H	0.24848700	1.75494800	-1.64882800
O	2.45253800	2.94596000	0.54298400
C	1.88974000	2.06326700	-0.17755600
O	-1.34962900	1.98775800	0.55861400
C	-2.19584700	1.05989100	0.39653200
C	-2.36966700	0.00815600	1.38239400
C	-3.03249100	0.99135700	-0.78875100
C	-3.28342200	-1.00296100	1.19780900
H	-1.75158400	0.04445500	2.27388400
C	-3.94267800	-0.02194500	-0.96400900
H	-2.91550000	1.77150100	-1.53417200
C	-4.07640300	-1.02872100	0.02433400
H	-4.56905700	-0.07536600	-1.84878000
H	-3.40341100	-1.78546600	1.94269100
O	-4.98681900	-1.99708900	-0.21225600
H	-5.00847600	-2.64330000	0.51066600

Geom 26:
Energy: -841.12648067 Hartrees

C	3.33964100	-2.06642300	-0.10876700
C	2.23776400	-1.65677900	-0.94764100
C	1.78217500	-0.35357600	-0.97577300
C	2.37003200	0.66721800	-0.17880800
C	3.45461800	0.28128800	0.65324800
C	3.92433900	-1.01485500	0.69443100
H	1.76596100	-2.41507100	-1.56833100
H	0.94839000	-0.11932200	-1.63038000
H	3.91704900	1.04602900	1.27069800
H	4.75737800	-1.27934100	1.34217400
O	3.76901000	-3.27030100	-0.07643900
C	0.82857600	2.47104800	-1.01188600
H	0.51264600	3.50683000	-0.97898300
H	0.30409500	1.80248500	-1.68007400
O	2.47681200	2.93211400	0.57489200
C	1.91855500	2.06747800	-0.17035400
O	-1.35547500	2.01169300	0.54027500
C	-2.19468500	1.07648000	0.38545900
C	-2.36529600	0.03469800	1.38245700
C	-3.02717300	0.98969800	-0.80159100
C	-3.27312300	-0.98333600	1.20687900
H	-1.75006300	0.08451100	2.27527400
C	-3.93125300	-0.03049400	-0.96790800
H	-2.91183200	1.76190400	-1.55550600
C	-4.06267300	-1.02654900	0.03159000
H	-4.55468900	-0.09754400	-1.85382400
H	-3.39085200	-1.75785700	1.96043500
O	-4.96762700	-2.00201600	-0.19662100
H	-4.98884100	-2.63990200	0.53366400

Geom 27:
Energy: -841.12733872 Hartrees

C	3.15927100	-1.98837600	-0.23767500
C	2.21797400	-1.43385800	-1.18220400
C	1.76084200	-0.13468400	-1.08506100
C	2.18969500	0.73933200	-0.04777300
C	3.11505600	0.20936100	0.89074800
C	3.58328800	-1.08535400	0.81013700
H	1.87017800	-2.07779800	-1.98677800
H	1.05321200	0.21332600	-1.83131000
H	3.45341600	0.85998300	1.69211500
H	4.29215500	-1.46276400	1.54412000

O	3.58817800	-3.18980500	-0.31876000
C	0.78983000	2.67328400	-0.83795700
H	0.46469600	3.69752500	-0.70222600
H	0.38553000	2.12126600	-1.67431200
O	2.14851700	2.86044400	1.05176400
C	1.73022600	2.12874900	0.10036900
O	-1.92436400	2.38793900	-0.37280100
C	-2.40613900	1.23915700	-0.14944800
C	-2.28416000	0.60390200	1.15065300
C	-3.09744400	0.48846500	-1.18333300
C	-2.79619200	-0.65045000	1.38612100
H	-1.77112600	1.15240900	1.93409900
C	-3.60469700	-0.76373000	-0.93914900
H	-3.19817900	0.95112800	-2.16004500
C	-3.45784100	-1.34649800	0.34467900
H	-4.11910000	-1.32821400	-1.71033000
H	-2.69807700	-1.11527800	2.36371500
O	-3.97573300	-2.58113500	0.51420500
H	-3.82374400	-2.90693300	1.41504200

Geom 28:
Energy: -841.12784551 Hartrees

C	3.18441100	-1.98448500	-0.22897000
C	2.23199400	-1.44132500	-1.16909100
C	1.77152700	-0.14299000	-1.07883500
C	2.20823100	0.74169400	-0.05375300
C	3.14505500	0.22319500	0.87994700
C	3.61615000	-1.07077900	0.80654800
H	1.87879400	-2.09335900	-1.96471500
H	1.05613800	0.19645300	-1.82159200
H	3.48954000	0.88226900	1.67172700
H	4.33313700	-1.43961200	1.53696400
O	3.61600100	-3.18520100	-0.30345300
C	0.78411000	2.65934000	-0.83931800
H	0.45562000	3.68338400	-0.70938100
H	0.36150500	2.09339100	-1.65728400
O	2.18236600	2.87699800	1.01836800
C	1.74714400	2.13131500	0.08573100
O	-1.97869000	2.40130000	-0.34500700
C	-2.44563100	1.24428400	-0.13346200
C	-2.32434100	0.60161300	1.16305400
C	-3.11922800	0.49150400	-1.17749300
C	-2.82232900	-0.66052600	1.38658800

H	-1.82355800	1.15119700	1.95366000
C	-3.61301800	-0.76829000	-0.94503700
H	-3.21847100	0.95919300	-2.15196200
C	-3.46884600	-1.35735000	0.33622600
H	-4.11496400	-1.33392700	-1.72354800
H	-2.72491400	-1.13095300	2.36154300
O	-3.97431600	-2.59859400	0.49465600
H	-3.82709300	-2.92726800	1.39526300

Geom 29:
Energy: -841.12828776 Hartrees

C	3.20411100	-1.98400900	-0.22124700
C	2.24126800	-1.45034900	-1.15632500
C	1.78052800	-0.15177800	-1.07316900
C	2.22771500	0.74290000	-0.06118300
C	3.17540000	0.23405800	0.86698300
C	3.64623200	-1.06030300	0.80111200
H	1.88074700	-2.10986000	-1.94242200
H	1.05782100	0.18053300	-1.81204900
H	3.52792700	0.90100400	1.64854700
H	4.37078400	-1.42201600	1.52759500
O	3.63570000	-3.18493600	-0.28900600
C	0.78200900	2.64678000	-0.83972000
H	0.45123000	3.67071500	-0.71404500
H	0.34031800	2.06786300	-1.63842600
O	2.22308800	2.89268200	0.98174000
C	1.76810800	2.13371500	0.06956500
O	-2.02749900	2.41539300	-0.30918700
C	-2.48184000	1.25087300	-0.11232200
C	-2.35393300	0.59349700	1.17611700
C	-3.14779600	0.50424500	-1.16564900
C	-2.84030800	-0.67574000	1.38439700
H	-1.85808600	1.13807100	1.97328900
C	-3.63037300	-0.76256000	-0.94828300
H	-3.25112600	0.98263100	-2.13448900
C	-3.48130700	-1.36542800	0.32598300
H	-4.12728800	-1.32325500	-1.73356900
H	-2.73817700	-1.15708500	2.35347900
O	-3.97688200	-2.61238900	0.46989800
H	-3.82828400	-2.95002200	1.36697400

Geom 30:
Energy: -841.12867072 Hartrees

C	3.22717600	-1.97799500	-0.21773000
C	2.25104500	-1.45442700	-1.14483400
C	1.78673300	-0.15702200	-1.06537200
C	2.24341100	0.74661200	-0.06551200
C	3.20475700	0.24802400	0.85424600
C	3.67893900	-1.04521100	0.79225900
H	1.88356200	-2.12075400	-1.92187400
H	1.05437600	0.16765200	-1.79811600
H	3.56475100	0.92200100	1.62629500
H	4.41339200	-1.39926300	1.51251800
O	3.66164000	-3.17793000	-0.28179000
C	0.77392300	2.63612700	-0.83345800
H	0.43942600	3.65925100	-0.71012500
H	0.31716800	2.04637900	-1.61571400
O	2.25185900	2.90713300	0.95490900
C	1.78142500	2.13696900	0.06023400
O	-2.08645800	2.42657800	-0.29308500
C	-2.52246200	1.25408400	-0.10251700
C	-2.38107100	0.59046300	1.18130700
C	-3.18077000	0.50458500	-1.15861200
C	-2.84946800	-0.68651900	1.38325100
H	-1.89015700	1.13685300	1.98029500
C	-3.64575200	-0.76979500	-0.94745600
H	-3.29334400	0.98733900	-2.12425000
C	-3.48511000	-1.37807500	0.32284100
H	-4.13754700	-1.33238900	-1.73460400
H	-2.73731500	-1.17258000	2.34885700
O	-3.96460600	-2.63192400	0.46104900
H	-3.81044500	-2.97226400	1.35616200

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p-cyanophenol leaving group

Geom 1:
C-O Bond Length: 1.48072 Angstrom
Energy: -858.14463 Hartrees

C	4.70748900	-1.39588200	-0.04214500
C	3.35363700	-1.73331300	-0.41826300
C	2.35365900	-0.78794300	-0.43866000
C	2.61805000	0.58493900	-0.10583500
C	3.96018300	0.92253600	0.28630400
C	4.96068500	-0.02464600	0.31360200
H	3.14182600	-2.76722100	-0.67782000
H	1.34881900	-1.09200900	-0.71059400
H	4.17657500	1.95031700	0.55348000
H	5.97195400	0.24650100	0.60596900
O	5.64025900	-2.29287900	-0.01799800
C	0.21008500	1.31784100	-0.62480700
H	-0.27440000	2.24467700	-0.94509800
H	0.18422300	0.59001600	-1.44192300
O	1.86703200	2.82487900	0.27993400
C	1.59309900	1.61690600	-0.14648700
O	-0.58121100	0.75635200	0.49372900
C	-1.87128300	0.38891400	0.27131000
C	-2.54322700	-0.18357100	1.36992900
C	-2.54052500	0.54874800	-0.95529300
C	-3.86103900	-0.59233900	1.24860100
H	-2.01239100	-0.29971500	2.30919000
C	-3.86507400	0.13654800	-1.07527300
H	-2.04606400	0.98902800	-1.81156800
C	-4.53608000	-0.43626600	0.01900600
H	-4.37509400	-1.03380500	2.09597400
H	-4.38276300	0.25959400	-2.02091900
C	-5.89230700	-0.85743500	-0.11275400
N	-7.00363400	-1.20348900	-0.21963100

Geom 2:
Bond Length: 1.53072 Angstrom
Energy: -858.144 Hartrees

C	4.72254500	-1.39188400	-0.03589800
C	3.37077200	-1.73495700	-0.41471900
C	2.36884900	-0.79156000	-0.44196800

C	2.62922200	0.58170100	-0.11491200
C	3.96704400	0.92512200	0.27990600
C	4.97106200	-0.01826800	0.31475700
H	3.16257000	-2.77054300	-0.67011000
H	1.36546500	-1.09932700	-0.71506800
H	4.17901600	1.95481400	0.54322300
H	5.98056900	0.25707300	0.60892400
O	5.65665600	-2.28496400	-0.00537500
C	0.22882800	1.31618400	-0.64909600
H	-0.26946700	2.23394000	-0.96836100
H	0.18954400	0.56537000	-1.44169500
O	1.86835900	2.81778200	0.28098400
C	1.59986600	1.61400900	-0.16265500
O	-0.59577900	0.75456900	0.51182000
C	-1.88179500	0.38796200	0.28251800
C	-2.56601000	-0.17409600	1.38079700
C	-2.54437400	0.53653400	-0.95047400
C	-3.88364100	-0.58106900	1.25352000
H	-2.04323400	-0.28300600	2.32550000
C	-3.86853600	0.12602900	-1.07652000
H	-2.04351100	0.96751100	-1.80776200
C	-4.54986800	-0.43522000	0.01774300
H	-4.40476000	-1.01351500	2.10133000
H	-4.37859900	0.24135300	-2.02733600
C	-5.90574200	-0.85424500	-0.12015600
N	-7.01726000	-1.19860200	-0.23216000

Geom 3:
Bond length: 1.58072 Angstrom
Energy: -858.1426 Hartrees

C	4.73595000	-1.38884200	-0.03200600
C	3.38477700	-1.73699200	-0.40878100
C	2.38181100	-0.79460600	-0.44113400
C	2.64073300	0.57896400	-0.12263900
C	3.97549500	0.92773600	0.27014500
C	4.98229500	-0.01250000	0.31085800
H	3.17848300	-2.77441700	-0.65774700
H	1.37862900	-1.10521400	-0.71168400
H	4.18466300	1.95954300	0.52741000
H	5.99120000	0.26647000	0.60324800
O	5.67049300	-2.27853900	0.00340900
C	0.24879600	1.31728700	-0.67017800
H	-0.26459300	2.22710100	-0.98309600

H	0.19637800	0.54775900	-1.44134600
O	1.87139000	2.81062500	0.28703600
C	1.60710100	1.61285700	-0.17578000
O	-0.60963700	0.75014300	0.52987500
C	-1.89158300	0.38544700	0.29457900
C	-2.58781000	-0.17021100	1.39055300
C	-2.54824700	0.52780900	-0.94386800
C	-3.90543200	-0.57443100	1.25631700
H	-2.07274900	-0.27566700	2.33994500
C	-3.87212500	0.11994500	-1.07696800
H	-2.04094200	0.95286800	-1.80036500
C	-4.56338600	-0.43377600	0.01535500
H	-4.43346600	-1.00084200	2.10301500
H	-4.37512700	0.23134500	-2.03208100
C	-5.91905000	-0.84965900	-0.12954900
N	-7.03091500	-1.19156400	-0.24732700

Geom 4:
Bond Length: 1.63072 Angstrom
Energy -858.1409 Hartrees

C	4.73924800	-1.39383000	-0.03280100
C	3.38580400	-1.74111600	-0.40309400
C	2.38613500	-0.79506900	-0.43748900
C	2.65119900	0.57730000	-0.12839600
C	3.98551200	0.92578100	0.25751800
C	4.99099200	-0.01566600	0.30103600
H	3.17605100	-2.77942600	-0.64488100
H	1.38082700	-1.10362600	-0.70241500
H	4.19727400	1.95883300	0.50768300
H	6.00156900	0.26231900	0.58804600
O	5.67019100	-2.28394700	0.00459200
C	0.27049500	1.33077100	-0.68453700
H	-0.25637600	2.23573500	-0.98434400
H	0.20185200	0.54758700	-1.43837800
O	1.88426400	2.80717400	0.29791200
C	1.61705900	1.61794800	-0.18383000
O	-0.62257800	0.75330800	0.55167400
C	-1.89891400	0.38783400	0.31019400
C	-2.60444800	-0.17428500	1.39913600
C	-2.55181500	0.53365500	-0.93171700
C	-3.92079200	-0.57878900	1.25537800
H	-2.09580700	-0.28381100	2.35161000
C	-3.87405400	0.12534800	-1.07443900

H	-2.04034400	0.96314800	-1.78359100
C	-4.57226100	-0.43372000	0.01127300
H	-4.45343100	-1.00916200	2.09729000
H	-4.37148000	0.24047300	-2.03212500
C	-5.92631400	-0.84970600	-0.14326800
N	-7.03746200	-1.19186900	-0.26887200

Geom 5:
Bond length: 1.68072 Angstrom
Energy: -858.1393 Hartrees

C	4.73187200	-1.40716300	-0.03831000
C	3.37307200	-1.74742000	-0.39678000
C	2.38117800	-0.79297900	-0.42984500
C	2.66036100	0.57677900	-0.13180500
C	3.99716500	0.91911300	0.24212800
C	4.99688600	-0.02814000	0.28510900
H	3.15416300	-2.78564300	-0.63014300
H	1.37118000	-1.09428700	-0.68510600
H	4.21704900	1.95248300	0.48406600
H	6.01152100	0.24389400	0.56283300
O	5.65515200	-2.30163600	-0.00217600
C	0.29422400	1.35655100	-0.69319100
H	-0.24372900	2.25944400	-0.97482500
H	0.20659500	0.56366000	-1.43292900
O	1.90691400	2.80738300	0.31301100
C	1.62998000	1.62920800	-0.18642000
O	-0.63476300	0.76577600	0.57676900
C	-1.90375000	0.39580400	0.32892100
C	-2.61527000	-0.18573200	1.40619900
C	-2.55519800	0.55380000	-0.91444500
C	-3.92894000	-0.59390200	1.25070700
H	-2.11147700	-0.30639400	2.36000600
C	-3.87428600	0.14154700	-1.06903000
H	-2.04204800	0.99764900	-1.75804300
C	-4.57607100	-0.43527900	0.00569900
H	-4.46352300	-1.03802400	2.08433300
H	-4.36784100	0.26749400	-2.02747400
C	-5.92710300	-0.85461900	-0.16065000
N	-7.03643400	-1.19969600	-0.29618300

Geom 6:
Bond length: 1.73072
Energy: -858.13807

C	4.71207800	-1.42958300	-0.04886000
C	3.34533000	-1.75535200	-0.39229700
C	2.36637300	-0.78739600	-0.42066300
C	2.66784300	0.57767700	-0.13289500
C	4.00971900	0.90671400	0.22613000
C	4.99856100	-0.05157500	0.26497100
H	3.11146300	-2.79192100	-0.61780600
H	1.34949500	-1.07512600	-0.66403500
H	4.24338800	1.93886400	0.46059600
H	6.01924800	0.20854700	0.53111800
O	5.62313800	-2.33300400	-0.01737200
C	0.32010900	1.39620600	-0.69675000
H	-0.22517900	2.30035000	-0.95517200
H	0.21040000	0.59773000	-1.42576900
O	1.93991100	2.81131100	0.33294600
C	1.64643400	1.64711600	-0.18309000
O	-0.64599200	0.78946800	0.60475700
C	-1.90563800	0.41005400	0.35015900
C	-2.61736200	-0.20748400	1.40976800
C	-2.55976500	0.59157000	-0.89103100
C	-3.92683600	-0.62314200	1.24090300
H	-2.11527600	-0.34850800	2.36180100
C	-3.87395200	0.17122300	-1.05926300
H	-2.04934300	1.06251400	-1.72166900
C	-4.57375200	-0.43901300	-0.00103800
H	-4.45903300	-1.09328100	2.06182700
H	-4.36692400	0.31716900	-2.01530300
C	-5.92034900	-0.86504300	-0.18065200
N	-7.02678000	-1.21576700	-0.32722900

Geom 7:
Bond length: 1.78072

Energy: -858.13738

C	4.67881200	-1.46193200	-0.06291000
C	3.30155800	-1.76619700	-0.38599900
C	2.34091300	-0.77989200	-0.40763700

C	2.67276200	0.57883300	-0.13247400
C	4.02252600	0.88782400	0.20686800
C	4.99510200	-0.08664100	0.23893300
H	3.04672000	-2.79977500	-0.60174900
H	1.31529900	-1.04852000	-0.63559800
H	4.27605300	1.91740200	0.43225700
H	6.02384400	0.15603100	0.48952300
O	5.57301300	-2.37888300	-0.03865300
C	0.34734000	1.44851500	-0.69618400
H	-0.19933700	2.35718000	-0.93051800
H	0.21073200	0.64616800	-1.41485100
O	1.98391800	2.81896400	0.35182600
C	1.66658300	1.67028000	-0.17604100
O	-0.65781700	0.83098000	0.63771600
C	-1.90538900	0.43483600	0.37517500
C	-2.61038100	-0.23399800	1.41055100
C	-2.56599600	0.64781300	-0.86012000
C	-3.91324700	-0.66320600	1.22625400
H	-2.10696000	-0.40175200	2.35766500
C	-3.87253300	0.21285200	-1.04430500
H	-2.06321400	1.15778300	-1.67241900
C	-4.56388300	-0.44541600	-0.00865200
H	-4.43811000	-1.17052800	2.02972600
H	-4.36799300	0.38527000	-1.99478100
C	-5.90346300	-0.88454700	-0.20379500
N	-7.00488200	-1.24607100	-0.36347700

Geom 8:
Bond length: 1.83072

Energy: -858.13734

C	4.15022300	-1.79714700	-0.10599600
C	2.71439600	-1.84745400	-0.28288000
C	1.95941500	-0.69614100	-0.29300700
C	2.56791700	0.58292900	-0.14786600
C	3.97740200	0.64615200	0.04543000
C	4.74948500	-0.49323000	0.06196600
H	2.25062900	-2.82283000	-0.39729700
H	0.88360900	-0.77102000	-0.40702900
H	4.44050300	1.61845700	0.17058200
H	5.82555200	-0.44138400	0.20012600
O	4.85248300	-2.86498200	-0.09001300

C	0.43210900	1.86026500	-0.65202100
H	0.02471600	2.84574600	-0.85095400
H	0.12067600	1.08750300	-1.34736600
O	2.31999000	2.91350500	0.32718800
C	1.77745300	1.84629200	-0.17485900
O	-0.64792800	1.40243600	0.75349000
C	-1.79892200	0.79639900	0.46995300
C	-2.30093500	-0.17590600	1.37526300
C	-2.55986000	1.08771200	-0.69203300
C	-3.50701100	-0.81553900	1.14083700
H	-1.72257000	-0.40676600	2.26472800
C	-3.76264400	0.43818200	-0.93278300
H	-2.20727700	1.83516900	-1.39401700
C	-4.25356100	-0.51950100	-0.02142600
H	-3.87978000	-1.55180100	1.84631600
H	-4.33591900	0.67338100	-1.82428800
C	-5.48910300	-1.18007500	-0.26955100
N	-6.50495500	-1.72453700	-0.47318500

Geom 9:
Bond length: 1.88072

Energy: -858.13783

C	4.06200300	-1.84601300	-0.10558100
C	2.62179600	-1.85465600	-0.25622000
C	1.90371600	-0.68022300	-0.27030300
C	2.55577800	0.57884900	-0.15261700
C	3.96869800	0.60306400	0.01484100
C	4.70574500	-0.55880600	0.03314000
H	2.12661500	-2.81672100	-0.34862800
H	0.82419300	-0.72042300	-0.36490500
H	4.46251000	1.56279400	0.11869100
H	5.78523700	-0.53957500	0.15060800
O	4.73029900	-2.93341200	-0.08776000
C	0.46855600	1.92355100	-0.67144800
H	0.07621100	2.91725700	-0.85513800
H	0.12373900	1.15138800	-1.35030000
O	2.37492200	2.91191200	0.32664300
C	1.80221600	1.86832300	-0.18087400
O	-0.65746900	1.49009100	0.77122300
C	-1.78588300	0.85215900	0.48748300
C	-2.25484000	-0.15831900	1.37105200
C	-2.56369600	1.14380000	-0.66564900

C	-3.44276900	-0.82779500	1.12776100
H	-1.66562200	-0.39246900	2.25263600
C	-3.74725200	0.46467700	-0.91593200
H	-2.23443500	1.91687300	-1.35167100
C	-4.20502300	-0.52785600	-0.02360000
H	-3.78976500	-1.59092500	1.81780300
H	-4.33219800	0.70193000	-1.79937800
C	-5.42187300	-1.21839800	-0.27954700
N	-6.42307700	-1.78757200	-0.48937100

Geom 10:
Bond length: 1.93072

Energy: -858.13863

C	3.97781600	-1.88912700	-0.10502500
C	2.53615400	-1.85925500	-0.24360800
C	1.85192100	-0.66499300	-0.26282800
C	2.54119100	0.57443700	-0.15961400
C	3.95492900	0.56232400	-0.00438600
C	4.65958400	-0.61897200	0.01722100
H	2.01390400	-2.80792700	-0.32368800
H	0.77104100	-0.67391400	-0.34945800
H	4.47520300	1.50926600	0.08717600
H	5.74015400	-0.62977400	0.12467400
O	4.61544700	-2.99310400	-0.08444900
C	0.50048600	1.98092500	-0.69341400
H	0.12413200	2.98255600	-0.86366300
H	0.12167300	1.21041400	-1.35473000
O	2.42316500	2.90869900	0.31985100
C	1.82307500	1.88675500	-0.19007200
O	-0.66897800	1.57681800	0.78872800
C	-1.77517000	0.90783600	0.50641300
C	-2.19586900	-0.15366800	1.35609300
C	-2.58324500	1.21320000	-0.62421300
C	-3.36381400	-0.85451400	1.10457500
H	-1.58537000	-0.40080000	2.21960800
C	-3.74605800	0.50361500	-0.88353400
H	-2.28892800	2.02266400	-1.28417100
C	-4.15503500	-0.53804200	-0.02285200
H	-3.67303900	-1.65552300	1.76928600
H	-4.35306300	0.75285400	-1.74869700
C	-5.35119400	-1.26042900	-0.28639500

N	-6.33591700	-1.85566600	-0.50279300

Geom 11:
Bond length: 1.98072

Energy: -858.13962

C	3.90421200	-1.92536400	-0.10217800
C	2.46449000	-1.86093100	-0.25316600
C	1.81061800	-0.65012300	-0.28024900
C	2.52975700	0.57098200	-0.17024400
C	3.94118300	0.52597000	-0.00462800
C	4.61665500	-0.67177400	0.02382100
H	1.92018200	-2.79674900	-0.33667300
H	0.73080300	-0.63173000	-0.37720600
H	4.48273500	1.46056700	0.09021400
H	5.69569500	-0.70949000	0.13962700
O	4.51450800	-3.04329500	-0.07535000
C	0.53192600	2.03160200	-0.71902600
H	0.16804300	3.04021300	-0.87136400
H	0.12303600	1.26626000	-1.36733400
O	2.46532700	2.90447600	0.31224000
C	1.84355200	1.90225300	-0.20222000
O	-0.67666300	1.64396300	0.80160400
C	-1.76490600	0.95177200	0.52155400
C	-2.14547200	-0.14740000	1.34415300
C	-2.59940400	1.26618100	-0.58912500
C	-3.29728300	-0.87242300	1.08741900
H	-1.51648100	-0.40331100	2.19180200
C	-3.74592300	0.53343100	-0.85383700
H	-2.33353000	2.10190600	-1.22857100
C	-4.11369400	-0.54476600	-0.01894800
H	-3.57494100	-1.70137400	1.73160300
H	-4.37210700	0.79070500	-1.70289200
C	-5.29274700	-1.29243900	-0.28721700
N	-6.26380000	-1.90856900	-0.50768800

Geom 12:
Bond length: 2.03072

Energy: -858.14066

C	3.84895900	-1.95265700	-0.09954500
C	2.41230500	-1.86072700	-0.26803600
C	1.78275000	-0.63743000	-0.30167900
C	2.52420300	0.56858700	-0.17889200
C	3.93228600	0.49741900	0.00262400
C	4.58429400	-0.71281800	0.03690800
H	1.85138600	-2.78585800	-0.35972200
H	0.70491300	-0.59755600	-0.41270100
H	4.48994900	1.42161500	0.10567300
H	5.66093300	-0.77181800	0.16516200
O	4.43743100	-3.08107000	-0.06763800
C	0.56287000	2.07060200	-0.74520400
H	0.20631600	3.08395600	-0.88010700
H	0.13110000	1.30952400	-1.38273400
O	2.49881700	2.90039400	0.30823500
C	1.86328700	1.91386800	-0.21251800
O	-0.68256900	1.68842600	0.81257100
C	-1.75734800	0.98110700	0.53311100
C	-2.11155900	-0.14217600	1.33692100
C	-2.60947300	1.30012000	-0.56458200
C	-3.25264900	-0.88242100	1.07666400
H	-1.47025100	-0.40339000	2.17375500
C	-3.74522100	0.55278900	-0.83275100
H	-2.36229100	2.15176200	-1.19073800
C	-4.08598600	-0.54804400	-0.01522200
H	-3.50955500	-1.72859200	1.70702200
H	-4.38401000	0.81452700	-1.67104000
C	-5.25407800	-1.31107500	-0.28653000
N	-6.21653700	-1.93986200	-0.50964700

Geom 13:
Bond length: 2.08072

Energy: -858.14169

C	3.78504900	-1.98346300	-0.09613600
C	2.35390300	-1.86029600	-0.29202200
C	1.75171600	-0.62366100	-0.33197700
C	2.51646600	0.56499700	-0.18698600
C	3.91883600	0.46374900	0.02072100
C	4.54415500	-0.76004300	0.06113500
H	1.77554300	-2.77286100	-0.39956300
H	0.67747900	-0.56002200	-0.46469700

H	4.49360600	1.37551400	0.13939900
H	5.61657000	-0.84297900	0.20973100
O	4.34886200	-3.12347400	-0.05946900
C	0.59696000	2.11080100	-0.77530500
H	0.25028000	3.12915600	-0.89563300
H	0.14252200	1.35443000	-1.40178900
O	2.53464700	2.89560500	0.30227000
C	1.88481700	1.92500200	-0.22461400
O	-0.68656000	1.73897500	0.81960300
C	-1.74711000	1.01487000	0.54195800
C	-2.07807800	-0.12422600	1.33549900
C	-2.61235500	1.32853300	-0.54864200
C	-3.20745100	-0.88138800	1.07381400
H	-1.42766400	-0.38299500	2.16612900
C	-3.73629100	0.56468800	-0.81808100
H	-2.38162300	2.18985700	-1.16811200
C	-4.05337500	-0.55039500	-0.00968500
H	-3.44618100	-1.73840000	1.69670900
H	-4.38426500	0.82316000	-1.65036200
C	-5.20956500	-1.33058700	-0.28173200
N	-6.16256000	-1.97359900	-0.50553300

Geom 14:
Bond length: -858.14169

Energy: -858.14267

C	3.72592700	-2.01120400	-0.09333900
C	2.30184300	-1.85904600	-0.31990400
C	1.72504100	-0.61070700	-0.36571300
C	2.50957900	0.56140000	-0.19503000
C	3.90478000	0.43208200	0.04233500
C	4.50527300	-0.80362400	0.08843900
H	1.70853500	-2.75952500	-0.44613900
H	0.65557600	-0.52549500	-0.52246300
H	4.49420000	1.33182900	0.17953600
H	5.57231900	-0.90850600	0.25993000
O	4.26677900	-3.16150700	-0.05209900
C	0.63056200	2.14759500	-0.80526600
H	0.29330400	3.17059600	-0.91090600
H	0.15548100	1.39711200	-1.42279000
O	2.56777000	2.89016500	0.29698200
C	1.90572200	1.93439700	-0.23663700
O	-0.68850700	1.78116600	0.82745300
C	-1.73702000	1.04373600	0.55098200

C	-2.04857300	-0.10835900	1.33554300
C	-2.61334800	1.35305500	-0.53351800
C	-3.16793400	-0.87940000	1.07234100
H	-1.39058500	-0.36509900	2.16089700
C	-3.72714300	0.57561200	-0.80431200
H	-2.39651300	2.22230900	-1.14715700
C	-4.02431000	-0.55124700	-0.00405700
H	-3.39138300	-1.74527800	1.68867800
H	-4.38270000	0.83128000	-1.63155000
C	-5.17035400	-1.34545000	-0.27724200
N	-6.11526400	-2.00012200	-0.50206400

Geom 15:
Bond length: 2.18072

Energy: -858.14358

C	3.68424800	-2.03047500	-0.09093500
C	2.26676600	-1.85747100	-0.34365500
C	1.70842600	-0.60106800	-0.39483000
C	2.50595500	0.55880700	-0.20278500
C	3.89454800	0.40923700	0.05994800
C	4.47698000	-0.83464600	0.11131900
H	1.66361700	-2.74902300	-0.48551200
H	0.64350200	-0.50073800	-0.57182600
H	4.49356500	1.30010700	0.21262600
H	5.53903600	-0.95521900	0.30222500
O	4.20830700	-3.18786200	-0.04543900
C	0.65887000	2.17548000	-0.83242500
H	0.32805000	3.20178400	-0.92493600
H	0.16604200	1.42958000	-1.44108700
O	2.59322400	2.88569600	0.29081600
C	1.92301300	1.94101100	-0.24807400
O	-0.69418600	1.81233400	0.83877800
C	-1.73290300	1.06517200	0.56189700
C	-2.02364400	-0.10399400	1.33085500
C	-2.62329400	1.37821500	-0.51136300
C	-3.13452800	-0.88583900	1.06451000
H	-1.35570400	-0.36460800	2.14701200
C	-3.72863900	0.59037700	-0.78509900
H	-2.42164100	2.25895400	-1.11392100
C	-4.00433600	-0.55277000	0.00019600

H	-3.34157000	-1.76405700	1.66906500
H	-4.39415000	0.84926800	-1.60337400
C	-5.14172600	-1.35791300	-0.27604300
N	-6.07970200	-2.02173300	-0.50351500

Geom 16:
Bond length: 2.23072

Energy: -858.14440847

C	3.66577500	-2.03941300	-0.08897700
C	2.25175400	-1.85530300	-0.35388200
C	1.70384700	-0.59459200	-0.40955700
C	2.50890400	0.55857400	-0.20921200
C	3.89403000	0.39838900	0.06532200
C	4.46631100	-0.84980800	0.12078800
H	1.64298400	-2.74207600	-0.50141300
H	0.64138200	-0.48597900	-0.59597200
H	4.49848200	1.28458400	0.22367800
H	5.52571300	-0.97889900	0.32054600
O	4.18042300	-3.20043500	-0.03987800
C	0.68046900	2.19161900	-0.85266200
H	0.35004800	3.21900800	-0.93393900
H	0.17401100	1.44665300	-1.45092700
O	2.61206000	2.88476600	0.28201500
C	1.93769600	1.94562200	-0.25779800
O	-0.70348600	1.82413200	0.85782100
C	-1.73584300	1.07336000	0.57633600
C	-2.00692500	-0.11818300	1.31932000
C	-2.64273000	1.40269100	-0.47927800
C	-3.11293600	-0.90438000	1.04634200
H	-1.32721400	-0.39206400	2.12133500
C	-3.74333000	0.61099800	-0.75945100
H	-2.45580300	2.29955400	-1.06267900
C	-3.99871000	-0.55404100	0.00071600
H	-3.30441400	-1.79922900	1.63138500
H	-4.42079400	0.88279100	-1.56364200
C	-5.13128100	-1.36337000	-0.28198400
N	-6.06550900	-2.03071900	-0.51488300

Geom 17:
Bond length: 2.28072

Energy: -858.14516801

C	3.80641900	-1.97274600	-0.08524500
C	2.37541200	-1.84896500	-0.28723700
C	1.77738500	-0.61160800	-0.34681700
C	2.54625700	0.57518100	-0.21241900
C	3.94765200	0.47522600	0.00075300
C	4.56962500	-0.74879400	0.05824100
H	1.79533400	-2.76152600	-0.38395600
H	0.70382400	-0.54645600	-0.48407100
H	4.52382300	1.38741900	0.10910400
H	5.64134300	-0.83331000	0.21025100
O	4.36689500	-3.11181700	-0.03290500
C	0.64290700	2.12388700	-0.84415000
H	0.26358600	3.13428300	-0.92485100
H	0.14948800	1.34625700	-1.41095700
O	2.56462300	2.90963800	0.24480800
C	1.91879000	1.93697300	-0.26676700
O	-0.73875900	1.71844600	0.92455500
C	-1.78458500	0.99964100	0.61781300
C	-2.01930900	-0.26976900	1.23489900
C	-2.74596500	1.44159500	-0.34513300
C	-3.13949800	-1.02478900	0.93324000
H	-1.29915800	-0.62983500	1.96431100
C	-3.86192400	0.68306600	-0.65352500
H	-2.58704800	2.39874400	-0.83355000
C	-4.07898300	-0.56165300	-0.01740800
H	-3.30200200	-1.98071700	1.42272200
H	-4.58079300	1.04166300	-1.38447100
C	-5.22672700	-1.33778200	-0.32988000
N	-6.17360100	-1.97763500	-0.58776900

Geom 18:
Bond length: 2.33072

Energy: -858.1458

C	3.78363100	-1.98619800	-0.08152200
C	2.35551700	-1.84778700	-0.29502400
C	1.77071600	-0.60440000	-0.35880900
C	2.55071500	0.57418300	-0.21676200
C	3.94921000	0.46014100	0.00809700
C	4.55817600	-0.77004300	0.06946800

H	1.76703600	-2.75434700	-0.39713500
H	0.69904500	-0.52825700	-0.50490800
H	4.53366200	1.36641000	0.12183800
H	5.62770500	-0.86567100	0.23001700
O	4.33223700	-3.13058900	-0.02611700
C	0.66944700	2.14254100	-0.86595000
H	0.29400900	3.15505700	-0.93911300
H	0.16452600	1.36667400	-1.42487400
O	2.58918600	2.90874400	0.23769700
C	1.93793200	1.94218000	-0.27578400
O	-0.74973200	1.73649300	0.93774900
C	-1.78847000	1.01201200	0.62726500
C	-2.01114100	-0.26668200	1.23129400
C	-2.75772100	1.45559400	-0.32814600
C	-3.12584700	-1.02766200	0.92518400
H	-1.28566500	-0.62854400	1.95456200
C	-3.86839600	0.69136000	-0.64044200
H	-2.60788500	2.41904200	-0.80712600
C	-4.07293500	-0.56212900	-0.01695500
H	-3.27871700	-1.99016400	1.40482900
H	-4.59293100	1.05160600	-1.36498800
C	-5.21539800	-1.34414700	-0.33325600
N	-6.15813300	-1.98896700	-0.59424000

Geom 19:
Bond length: 2.38072

Energy: -858.14632

C	3.67529300	-2.03925800	-0.07967000
C	2.26280000	-1.84769300	-0.34928500
C	1.72417700	-0.58384300	-0.41749600
C	2.53757600	0.56454900	-0.22401800
C	3.92094200	0.39798500	0.05572000
C	4.48428700	-0.85327900	0.12234000
H	1.64821800	-2.73146200	-0.49022400
H	0.66286400	-0.46926700	-0.60679300
H	4.53108800	1.28140000	0.20781200
H	5.54233600	-0.98843200	0.32497100
O	4.18177900	-3.20248700	-0.02054800
C	0.72893100	2.20704600	-0.90056900
H	0.38577500	3.23196800	-0.96067600
H	0.19752500	1.45325500	-1.46492200
O	2.65193000	2.89381700	0.24504700

C	1.97680700	1.95451600	-0.28554400
O	-0.74582700	1.81400600	0.92657400
C	-1.76795700	1.06614300	0.62314500
C	-1.98127200	-0.19904900	1.25984700
C	-2.73157500	1.46832000	-0.35714800
C	-3.08082000	-0.98407400	0.96088800
H	-1.26063400	-0.53008800	2.00248800
C	-3.82692000	0.67970100	-0.66194400
H	-2.58867900	2.42002100	-0.86120000
C	-4.02209300	-0.55896400	-0.00608600
H	-3.22644300	-1.93477600	1.46566600
H	-4.54677900	1.00884000	-1.40570900
C	-5.14909200	-1.36592700	-0.31410400
N	-6.07926200	-2.03159500	-0.56806600

Geom 20:
Bond length: 2.43072

Energy: -858.14673

C	3.62620300	-2.06315100	-0.07385400
C	2.21781600	-1.84821100	-0.34781400
C	1.70081500	-0.57551600	-0.41961400
C	2.53324800	0.55883700	-0.22513200
C	3.91250600	0.36960200	0.06067500
C	4.45451900	-0.89072700	0.13016200
H	1.58887100	-2.72168900	-0.48943900
H	0.64220200	-0.44318500	-0.61244200
H	4.53676400	1.24294500	0.21374700
H	5.50950000	-1.04358400	0.33607500
O	4.11306500	-3.23441000	-0.01280000
C	0.76455200	2.23296600	-0.92947500
H	0.43656000	3.26295700	-0.98953600
H	0.21980500	1.48506900	-1.48914300
O	2.68199500	2.88594200	0.24313800
C	1.99779600	1.95802900	-0.29368600
O	-0.76798100	1.87729900	0.92343100
C	-1.77362000	1.10811000	0.62350400
C	-1.95393900	-0.16648800	1.25306800
C	-2.75392100	1.49398600	-0.34766100
C	-3.03626800	-0.97520300	0.95519500
H	-1.22073600	-0.48588900	1.98848900
C	-3.83260900	0.68231100	-0.65045900

H	-2.63606500	2.45215600	-0.84605700
C	-3.99397700	-0.56562300	-0.00254900
H	-3.15603300	-1.93275700	1.45376500
H	-4.56521000	0.99954100	-1.38694100
C	-5.10323100	-1.39684800	-0.30980500
N	-6.01880500	-2.08266500	-0.56342800

Geom 21:
Bond length: 2.48072

Energy: -858.14708607

C	3.57973300	-2.08399000	-0.06567400
C	2.17523000	-1.84771100	-0.34254200
C	1.67858700	-0.56723900	-0.42005100
C	2.52898400	0.55410600	-0.22835300
C	3.90439700	0.34420500	0.06170400
C	4.42631000	-0.92418300	0.13629400
H	1.53269100	-2.71160500	-0.48180500
H	0.62249300	-0.41892200	-0.61510500
H	4.54200500	1.20818600	0.21287700
H	5.47836300	-1.09307800	0.34453700
O	4.04780200	-3.26245400	-0.00037000
C	0.79552200	2.25588400	-0.95535700
H	0.48268300	3.29063400	-1.01666300
H	0.23706600	1.51352100	-1.50901200
O	2.71220700	2.87981700	0.23258800
C	2.01741200	1.96136200	-0.30522700
O	-0.79337000	1.93956600	0.92330100
C	-1.78249100	1.14949300	0.62656100
C	-1.91941800	-0.14111900	1.23524000
C	-2.78870000	1.52582400	-0.32237100
C	-2.98256300	-0.97445600	0.93672100
H	-1.16650900	-0.45389900	1.95338500
C	-3.84901000	0.69036200	-0.62471700
H	-2.70472300	2.49608400	-0.80405300
C	-3.96552900	-0.57411300	0.00063100
H	-3.06798300	-1.94451200	1.41784800
H	-4.60119100	1.00063400	-1.34424400
C	-5.05445600	-1.43099500	-0.30846400
N	-5.95315100	-2.13815200	-0.56404000

Geom 22:
Bond length: 2.53072

Energy: -858.14736

C	3.55389600	-2.09484600	-0.06001400
C	2.15466300	-1.84582400	-0.35245500
C	1.67055000	-0.56096100	-0.43608200
C	2.52909600	0.55253800	-0.23518400
C	3.89929200	0.33021800	0.07024900
C	4.40882200	-0.94271900	0.15099600
H	1.50585900	-2.70388000	-0.49849000
H	0.61803900	-0.40357400	-0.64292400
H	4.54291300	1.18845900	0.22832700
H	5.45691000	-1.12105900	0.37094900
O	4.01017200	-3.27742200	0.01080100
C	0.81873300	2.27178900	-0.97921400
H	0.51362600	3.30921400	-1.03711000
H	0.25051000	1.53367000	-1.52871200
O	2.73233100	2.87723100	0.22107300
C	2.03248700	1.96441700	-0.31822900
O	-0.80233500	1.95811200	0.93867800
C	-1.78503600	1.16273700	0.63856900
C	-1.90185600	-0.14048600	1.22528900
C	-2.80568500	1.54419600	-0.29347800
C	-2.95768200	-0.98088900	0.92119500
H	-1.13842800	-0.45736900	1.93041700
C	-3.85898100	0.70197700	-0.60080900
H	-2.73801800	2.52413300	-0.75788400
C	-3.95441800	-0.57538100	0.00186500
H	-3.02683600	-1.96075600	1.38474700
H	-4.62173800	1.01634500	-1.30733200
C	-5.03550000	-1.43966600	-0.31349600
N	-5.92778200	-2.15302000	-0.57451700

Geom 23:
Bond length: 2.58072
Energy: -858.14757

C	3.52876200	-2.10464900	-0.05414900
C	2.13729700	-1.84421800	-0.37280400
C	1.66454300	-0.55555700	-0.46274800
C	2.52753200	0.55085500	-0.24261400

C	3.88995100	0.31726000	0.08855800
C	4.38820500	-0.95957200	0.17615500
H	1.48499800	-2.69695200	-0.53361800
H	0.61739700	-0.39048900	-0.68966700
H	4.53676200	1.17024100	0.26122600
H	5.43046400	-1.14631900	0.41587000
O	3.97439800	-3.29075300	0.02231100
C	0.84062300	2.28618600	-1.00666800
H	0.54380400	3.32625500	-1.06327600
H	0.26417300	1.55240600	-1.55351900
O	2.74797300	2.87466800	0.20962300
C	2.04498000	1.96689400	-0.33263400
O	-0.81119100	1.97833700	0.95212500
C	-1.78709900	1.17673100	0.64962100
C	-1.88307800	-0.13758700	1.21601800
C	-2.82216400	1.56094800	-0.26587000
C	-2.93124300	-0.98580200	0.90763300
H	-1.10894100	-0.45678100	1.90831800
C	-3.86809200	0.71117900	-0.57690800
H	-2.77116000	2.54938100	-0.71419600
C	-3.94191200	-0.57744900	0.00473000
H	-2.98371100	-1.97428200	1.35482600
H	-4.64161000	1.02790700	-1.27058600
C	-5.01480400	-1.44993300	-0.31548700
N	-5.90037300	-2.17015600	-0.58069100

Geom 24:
Bond length: 2.63072
Energy: -858.14772

C	3.47729200	-2.12507400	-0.05151400
C	2.10430300	-1.84011300	-0.42461000
C	1.65496300	-0.54364800	-0.52152000
C	2.52441300	0.54770700	-0.25547500
C	3.86918500	0.28961500	0.12660000
C	4.34403200	-0.99537900	0.22311100
H	1.44640900	-2.68113000	-0.62044200
H	0.62052200	-0.36231300	-0.78989300
H	4.52129200	1.13090300	0.33307100
H	5.37277300	-1.20010100	0.50313500
O	3.90070300	-3.31856500	0.03289800
C	0.87646000	2.31707300	-1.03342300
H	0.59647700	3.36246500	-1.08096800
H	0.28611400	1.59724700	-1.58390100

O	2.78033900	2.86676600	0.20301200
C	2.06813400	1.97207900	-0.34772200
O	-0.79767700	1.98559600	0.96860000
C	-1.77222900	1.18467700	0.66306700
C	-1.85856300	-0.13824600	1.21171200
C	-2.81668800	1.57712700	-0.23876800
C	-2.90538200	-0.98652200	0.89947400
H	-1.07763000	-0.46378100	1.89336600
C	-3.86134200	0.72734200	-0.55334900
H	-2.77345800	2.57204000	-0.67342100
C	-3.92503000	-0.56989400	0.01040200
H	-2.94999200	-1.98155900	1.33278100
H	-4.64173500	1.05041200	-1.23634300
C	-4.99645200	-1.44248000	-0.31391400
N	-5.88089800	-2.16287800	-0.58255600

Geom 25:
Bond length: 2.68072
Geometry: -858.14791

C	2.60898600	-2.39654000	-0.09890600
C	1.73211000	-1.78755200	-1.08131600
C	1.62494700	-0.41956100	-1.17877900
C	2.37323100	0.43208700	-0.32345600
C	3.24695200	-0.14567500	0.63867900
C	3.36480000	-1.50809400	0.76214100
H	1.16815700	-2.44515000	-1.73563800
H	0.96858600	0.00511100	-1.92947400
H	3.81535700	0.51272300	1.28610900
H	4.02153600	-1.95499900	1.50225500
O	2.71024400	-3.65846500	0.00008600
C	1.20639100	2.54981200	-1.08534000
H	1.17166900	3.63359800	-1.09952700
H	0.43263700	2.00228700	-1.60467400
O	3.17836800	2.61695600	0.16553700
C	2.28401200	1.92311300	-0.40697200
O	-0.33848300	2.03423600	1.04393800
C	-1.34920600	1.28505800	0.73127700
C	-1.49006800	-0.04382500	1.25534400
C	-2.38196900	1.74372200	-0.15334300
C	-2.57921500	-0.83511000	0.93933500
H	-0.71933500	-0.41775800	1.92342100

C	-3.46821500	0.95025200	-0.47171700
H	-2.29448800	2.74316900	-0.57015600
C	-3.58650900	-0.35277300	0.06996400
H	-2.66690500	-1.83522400	1.35380900
H	-4.23943400	1.32150800	-1.14033300
C	-4.70227200	-1.16724900	-0.25749800
N	-5.62323800	-1.83901100	-0.52839400

Geom 26:
Bond length: 2.73072
Energy: -858.14804

C	2.37536800	-2.46463700	-0.11588900
C	1.56734200	-1.78237100	-1.10896000
C	1.57148300	-0.40971100	-1.20024500
C	2.36903500	0.37553700	-0.32671600
C	3.17926300	-0.27519400	0.64441200
C	3.18633300	-1.64315200	0.76134000
H	0.96419900	-2.38943100	-1.77704900
H	0.96438500	0.06941300	-1.95985000
H	3.78701700	0.33358000	1.30468400
H	3.79345600	-2.14429900	1.50908300
O	2.37146700	-3.73123500	-0.02112200
C	1.37455100	2.57544000	-1.08805200
H	1.41317900	3.65935800	-1.08913800
H	0.57039600	2.08622600	-1.61942000
O	3.32535400	2.49076000	0.19614700
C	2.39371900	1.86780800	-0.39710800
O	-0.21820200	2.02248000	1.06002200
C	-1.24941100	1.30627500	0.74171700
C	-1.42458000	-0.02589300	1.24873000
C	-2.27307200	1.80585500	-0.13207400
C	-2.53769300	-0.78127300	0.92885300
H	-0.66111300	-0.42995900	1.90738400
C	-3.38293800	1.04800500	-0.45404400
H	-2.15906000	2.80780000	-0.53618200
C	-3.53518200	-0.25819200	0.07193900
H	-2.65217800	-1.78391300	1.33039900
H	-4.14715300	1.44931000	-1.11320600
C	-4.67645000	-1.03539000	-0.25890300
N	-5.61838500	-1.67611000	-0.53244100

Geom 27:
Bond length: 2.78072

Energy: -858.14822

C	2.14132100	-2.52360100	-0.14855800
C	1.36869300	-1.75971900	-1.10913400
C	1.48754800	-0.39115300	-1.18476900
C	2.36896000	0.31388100	-0.32348500
C	3.14540600	-0.42015400	0.61653800
C	3.04197000	-1.78560100	0.71436900
H	0.69599700	-2.30233300	-1.76627400
H	0.89626500	0.14467500	-1.91797500
H	3.81948000	0.12356000	1.26918200
H	3.62583300	-2.34622600	1.43816300
O	2.02989200	-3.78706400	-0.06812400
C	1.59241500	2.59872200	-1.09617800
H	1.71173300	3.67620800	-1.05845500
H	0.79243600	2.19017000	-1.69780500
O	3.45000300	2.34286400	0.29358600
C	2.51056000	1.79866500	-0.36212400
O	-0.07733200	1.97826000	1.03909500
C	-1.13992200	1.30923800	0.72885800
C	-1.36440200	-0.01844100	1.23099000
C	-2.15204200	1.85840000	-0.12987300
C	-2.51306000	-0.72303700	0.92164500
H	-0.61049100	-0.45739500	1.87788400
C	-3.29699900	1.15094100	-0.44049900
H	-1.99946300	2.85677300	-0.52984200
C	-3.49721000	-0.15105600	0.08110200
H	-2.66623800	-1.72218600	1.31868600
H	-4.05248600	1.58763600	-1.08694800
C	-4.67585700	-0.87586500	-0.23883500
N	-5.64826400	-1.47295300	-0.50333500

Geom 28:
Bond length: 2.83072
Energy: -858.14838

C	2.08289500	-2.52915800	-0.15156800
C	1.33597200	-1.75310200	-1.12241200
C	1.48107900	-0.38705200	-1.19990600
C	2.36462700	0.30401800	-0.32979800
C	3.11650500	-0.44255400	0.62053500
C	2.98650100	-1.80551800	0.72014200
H	0.66145900	-2.28460300	-1.78677100
H	0.90855900	0.15780900	-1.94135600
H	3.79305000	0.08981900	1.28004100
H	3.55140700	-2.37486300	1.45217900
O	1.94758000	-3.79060400	-0.06989500
C	1.63610300	2.60126800	-1.11230700
H	1.77846400	3.67615900	-1.07844300
H	0.82557800	2.20776400	-1.71021700
O	3.48146200	2.31387700	0.28677100
C	2.53523600	1.78445700	-0.37094500
O	-0.02785600	1.92249700	1.07481700
C	-1.10370000	1.28143000	0.75445500
C	-1.34786500	-0.05658500	1.21957400
C	-2.11185200	1.87347700	-0.08079700
C	-2.50988200	-0.73239400	0.89611800
H	-0.59797500	-0.52654200	1.84899100
C	-3.27004600	1.19489000	-0.40489200
H	-1.94413400	2.88042900	-0.45206700
C	-3.48845300	-0.11901700	0.07877900
H	-2.67782500	-1.74016400	1.26420300
H	-4.02200700	1.66294400	-1.03320500
C	-4.68048600	-0.81463400	-0.25662600
N	-5.66369500	-1.38743700	-0.53414400

Geom 29:
Bond length: 2.88072
Energy: -858.14874

C	1.02816200	-2.62037600	-0.24951800
C	0.79716300	-1.66578000	-1.31504800
C	1.43472700	-0.44631900	-1.32638000
C	2.33599400	-0.08248300	-0.29189700
C	2.58858100	-1.01287200	0.75378400
C	1.95807100	-2.23247300	0.79125600
H	0.10895800	-1.94581000	-2.10692100
H	1.24114500	0.23854200	-2.14423300
H	3.27898200	-0.73297100	1.54220600
H	2.13913000	-2.93570100	1.59883900

O	0.44151300	-3.75022100	-0.23223600
C	2.51751100	2.32347600	-1.03824400
H	3.00331300	3.28900600	-0.94300000
H	1.68239700	2.23013400	-1.71915200
O	4.00931600	1.41260500	0.51091800
C	3.01184400	1.24095700	-0.25312200
O	0.47002400	1.96554500	0.95631200
C	-0.67812000	1.44898900	0.67526200
C	-1.15458400	0.26939100	1.34724500
C	-1.54198500	2.02904600	-0.31724300
C	-2.40274600	-0.25931900	1.07605600
H	-0.51426700	-0.18935800	2.09458400
C	-2.78576700	1.49546400	-0.58827600
H	-1.19524000	2.91101500	-0.84782500
C	-3.23676800	0.34524700	0.10663000
H	-2.75044800	-1.14248000	1.60333500
H	-3.42831100	1.95246800	-1.33482100
C	-4.52000600	-0.19800400	-0.17197500
N	-5.57784900	-0.64399200	-0.40202200

Geom 30:
Bond length: 2.93072
Energy: -858.14895

C	0.98950800	-2.61180400	-0.24798800
C	0.76885300	-1.65299200	-1.31177100
C	1.42659500	-0.44416400	-1.32612400
C	2.33891500	-0.09554400	-0.29627700
C	2.58053900	-1.02993900	0.74842500
C	1.92988300	-2.23884700	0.78878600
H	0.07266900	-1.92134800	-2.10071800
H	1.24087900	0.24330600	-2.14361800
H	3.27930200	-0.76167100	1.53356500
H	2.10312600	-2.94503400	1.59552000
O	0.38593500	-3.73288400	-0.22897300
C	2.56040700	2.30658600	-1.04563300
H	3.06877600	3.26117600	-0.95798900
H	1.71358800	2.23128200	-1.71445600
O	4.04536800	1.36850100	0.49339900
C	3.03920200	1.21462200	-0.26297100
O	0.47679200	1.95835000	0.98572600

C	-0.67149400	1.44909900	0.69495200
C	-1.15814300	0.26789900	1.35746100
C	-1.52621500	2.03901700	-0.30018800
C	-2.40674600	-0.25350400	1.07468300
H	-0.52501800	-0.19768000	2.10667500
C	-2.77033500	1.51270600	-0.58257500
H	-1.17149800	2.92222500	-0.82335400
C	-3.23111000	0.36046700	0.10291700
H	-2.76223800	-1.13792800	1.59454500
H	-3.40591500	1.97652500	-1.33086000
C	-4.51471800	-0.17564200	-0.18785400
N	-5.57275200	-0.61576400	-0.42794000

Phenol as a leaving group:

Geom 1:
Energy: -765.88607390

C	4.16179100	-1.16285900	-0.05917800
C	2.83965600	-1.59067600	-0.46214100
C	1.76274000	-0.73246100	-0.45571900
C	1.90666100	0.64700400	-0.06947100
C	3.21542200	1.07443600	0.35605700
C	4.29011700	0.21128500	0.35618900
H	2.71723200	-2.62809100	-0.76344000
H	0.78704400	-1.10823000	-0.74459500
H	3.33189900	2.10570900	0.66858600
H	5.27331700	0.55117500	0.67316700
O	5.16168100	-1.97577000	-0.06106700
C	-0.54503800	1.19455100	-0.58757700
H	-1.10390400	2.09570200	-0.86056500
H	-0.49898000	0.52272700	-1.45421300
O	0.98360100	2.80426300	0.36202000
C	0.80942700	1.59742700	-0.08728300
O	-1.27997500	0.49746700	0.47779700
C	-2.54364100	0.04654100	0.22138400
C	-3.17284200	-0.64673400	1.27191500
C	-3.22713900	0.23461300	-0.99055300
C	-4.46495300	-1.14189600	1.11112100
H	-2.63233900	-0.78536400	2.20349600
C	-4.52620500	-0.27101800	-1.13666500
H	-2.76815600	0.76633400	-1.81492800
C	-5.15365700	-0.95837200	-0.09648100
H	-4.93688500	-1.67448200	1.93222700
H	-5.04523400	-0.11906400	-2.07913400
H	-6.16048100	-1.34513700	-0.22019400

Geom 2:
Energy: -765.88532846

C	4.16179100	-1.16285900	-0.05917800
C	2.83965600	-1.59067600	-0.46214100
C	1.76274000	-0.73246100	-0.45571900

C	1.90666100	0.64700400	-0.06947100
C	3.21542200	1.07443600	0.35605700
C	4.29011700	0.21128500	0.35618900
H	2.71723200	-2.62809100	-0.76344000
H	0.78704400	-1.10823000	-0.74459500
H	3.33189900	2.10570900	0.66858600
H	5.27331700	0.55117500	0.67316700
O	5.16168100	-1.97577000	-0.06106700
C	-0.54503800	1.19455100	-0.58757700
H	-1.10390400	2.09570200	-0.86056500
H	-0.49898000	0.52272700	-1.45421300
O	0.98360100	2.80426300	0.36202000
C	0.80942700	1.59742700	-0.08728300
O	-1.27997500	0.49746700	0.47779700
C	-2.54364100	0.04654100	0.22138400
C	-3.17284200	-0.64673400	1.27191500
C	-3.22713900	0.23461300	-0.99055300
C	-4.46495300	-1.14189600	1.11112100
H	-2.63233900	-0.78536400	2.20349600
C	-4.52620500	-0.27101800	-1.13666500
H	-2.76815600	0.76633400	-1.81492800
C	-5.15365700	-0.95837200	-0.09648100
H	-4.93688500	-1.67448200	1.93222700
H	-5.04523400	-0.11906400	-2.07913400
H	-6.16048100	-1.34513700	-0.22019400

Geom 3:
Energy: -765.88365468

C	4.17183400	-1.17184800	-0.05212100
C	2.84978200	-1.59823400	-0.45813700
C	1.77698500	-0.73446500	-0.45982200
C	1.92583400	0.64317700	-0.08241200
C	3.22966200	1.06907100	0.34620500
C	4.30337700	0.20446600	0.35651900
H	2.72492600	-2.63681300	-0.75358400
H	0.80051500	-1.10789200	-0.74902500
H	3.34629200	2.10184300	0.65372000
H	5.28603900	0.54315400	0.67561700
O	5.16670600	-1.98566700	-0.04574800
C	-0.50669300	1.21852700	-0.62247100
H	-1.08459000	2.10446800	-0.89108900

H	-0.49069100	0.49918000	-1.44510800
O	1.00696600	2.79946200	0.37101700
C	0.82817100	1.60385200	-0.10969300
O	-1.31390300	0.51150600	0.52366500
C	-2.56467200	0.05564400	0.24405200
C	-3.21891800	-0.63505800	1.28454000
C	-3.22959200	0.23086700	-0.98276600
C	-4.50625000	-1.13489200	1.10078400
H	-2.69881400	-0.76744200	2.22875000
C	-4.52344900	-0.27975100	-1.15237200
H	-2.75778300	0.75910100	-1.80219000
C	-5.17167300	-0.96236700	-0.12141900
H	-4.99282700	-1.66358500	1.91612400
H	-5.02302300	-0.13522300	-2.10666500
H	-6.17458400	-1.35313200	-0.26335000

Geom 4:
Energy: -765.88159396

C	4.15741700	-1.19160900	-0.05576900
C	2.82852200	-1.60710600	-0.45174100
C	1.76587100	-0.73071900	-0.45287300
C	1.93293800	0.64541900	-0.08615300
C	3.24074700	1.06094300	0.33203000
C	4.30637800	0.18645900	0.34284800
H	2.69112300	-2.64621700	-0.73913200
H	0.78330200	-1.09461100	-0.73334500
H	3.36897000	2.09469800	0.63162100
H	5.29427400	0.51692800	0.65376300
O	5.14208800	-2.01426200	-0.04962700
C	-0.48574500	1.25589000	-0.62889100
H	-1.06939300	2.13930700	-0.88748300
H	-0.49153400	0.51864600	-1.43320700
O	1.03524500	2.80679200	0.38750500
C	0.84199600	1.62139600	-0.11298600
O	-1.33233100	0.54270500	0.55401200
C	-2.56974500	0.07077100	0.25974200
C	-3.22652100	-0.64318300	1.28492500
C	-3.22930000	0.24950600	-0.97122500
C	-4.50501200	-1.15885200	1.08334200
H	-2.71406200	-0.78042000	2.23272800
C	-4.51355900	-0.27787400	-1.15924700

H	-2.75898400	0.79557700	-1.77986400
C	-5.16207500	-0.98216000	-0.14280800
H	-4.99114500	-1.70423500	1.88806000
H	-5.00627200	-0.12900100	-2.11657100
H	-6.15777700	-1.38584600	-0.29885600

Geom 5:
Energy: -765.87958217 Hartrees

C	4.11939700	-1.22718700	-0.06805900
C	2.77850800	-1.61856800	-0.44938000
C	1.73486600	-0.71944700	-0.44548100
C	1.93502800	0.65227800	-0.08827400
C	3.25205200	1.04495600	0.31378800
C	4.30095700	0.15076500	0.32039400
H	2.61767100	-2.65627600	-0.72902200
H	0.74192300	-1.06336100	-0.71428800
H	3.40231500	2.07816300	0.60513800
H	5.29826600	0.46302700	0.61916200
O	5.08551200	-2.06775900	-0.06598800
C	-0.46434600	1.32273100	-0.62486700
H	-1.04769500	2.21020400	-0.86403900
H	-0.50099200	0.57428300	-1.41583800
O	1.08075900	2.82400900	0.41605400
C	0.85989600	1.65438100	-0.10800600
O	-1.35179300	0.60191300	0.59249300
C	-2.56745300	0.09782700	0.28063400
C	-3.20721300	-0.67500000	1.27574600
C	-3.23247700	0.29799900	-0.94611200
C	-4.46870900	-1.22235300	1.05104500
H	-2.69405300	-0.83121000	2.22036800
C	-4.49814600	-0.26313200	-1.15854300
H	-2.77878900	0.88991900	-1.73193900
C	-5.12779900	-1.02366000	-0.17069400
H	-4.93959100	-1.81118900	1.83410700
H	-4.99259800	-0.09542300	-2.11200600
H	-6.10965200	-1.45297600	-0.34525300

Geom 6:

Energy: -765.87792966 Hartrees

C	4.03012600	-1.29020500	-0.09666000
C	2.67152200	-1.62893400	-0.46780200
C	1.66462400	-0.68896600	-0.45156100
C	1.92239200	0.66972500	-0.09043100
C	3.25427300	1.01150500	0.30020100
C	4.26909200	0.07919000	0.29480900
H	2.46862900	-2.65846500	-0.74981100
H	0.65653800	-0.99160700	-0.71341000
H	3.44470400	2.03735400	0.59448500
H	5.28024500	0.35153000	0.58537900
O	4.96145300	-2.16529000	-0.10611700
C	-0.44615400	1.44423200	-0.60425800
H	-1.01649200	2.34685600	-0.80920500
H	-0.53465700	0.69424100	-1.38797800
O	1.15595200	2.86475600	0.44930800
C	0.88259300	1.71749900	-0.09480500
O	-1.37209300	0.71661900	0.64946800
C	-2.54739500	0.14700500	0.31575100
C	-3.10955400	-0.76592500	1.23849700
C	-3.25612600	0.41360900	-0.87560800
C	-4.33497100	-1.37825500	0.98168400
H	-2.56546500	-0.97615500	2.15505700
C	-4.48181100	-0.21598500	-1.12356600
H	-2.86421200	1.11495400	-1.60317600
C	-5.03383800	-1.11239200	-0.20461400
H	-4.74539300	-2.07248400	1.71078900
H	-5.00892000	0.00641300	-2.04806400
H	-5.98612100	-1.59392500	-0.40516600

Geom 7:
Energy: -765.87687198 Hartrees

C	3.95108200	-1.34271600	-0.11282500
C	2.57349200	-1.64387400	-0.44720900
C	1.59950300	-0.67003000	-0.42446400
C	1.91164100	0.68247300	-0.09230400
C	3.26000500	0.98890600	0.26109100
C	4.24458600	0.02541500	0.24923700
H	2.33118000	-2.67077000	-0.70624600
H	0.57549600	-0.94128500	-0.65719000
H	3.48845900	2.01312700	0.53340200
H	5.27074000	0.26864000	0.51104500

O	4.85181100	-2.24551700	-0.12820900
C	-0.42627100	1.53957600	-0.59445200
H	-0.98752900	2.45125700	-0.77716800
H	-0.55586600	0.78173600	-1.36316000
O	1.21936000	2.89670200	0.46316900
C	0.90173700	1.76752900	-0.08812400
O	-1.39551700	0.81502800	0.69733300
C	-2.53137600	0.18945500	0.34635200
C	-3.03150500	-0.81290200	1.21262300
C	-3.26977700	0.48329500	-0.82296800
C	-4.22267200	-1.47863200	0.92692000
H	-2.46764700	-1.04732300	2.11140300
C	-4.45771600	-0.20132500	-1.10266200
H	-2.92608700	1.25270900	-1.50553000
C	-4.94776500	-1.18333500	-0.23643500
H	-4.58495500	-2.23890200	1.61473100
H	-5.00651300	0.04522000	-2.00840000
H	-5.87230400	-1.70711700	-0.45991600

Geom 8:
Energy: -765.87638027 Hartrees

C	3.80919700	-1.42252900	-0.12916100
C	2.40231400	-1.66414800	-0.38247300
C	1.48318700	-0.63859500	-0.35361500
C	1.88298000	0.70483800	-0.09424400
C	3.25922900	0.95529600	0.17952500
C	4.19199600	-0.05749700	0.15988600
H	2.09524700	-2.68633400	-0.58445200
H	0.43492600	-0.86041900	-0.52131800
H	3.55311100	1.97604900	0.39697500
H	5.24150600	0.14023300	0.35922800
O	4.65978900	-2.36932800	-0.15029800
C	-0.40725700	1.67764600	-0.58011500
H	-0.94671300	2.60545900	-0.73977000
H	-0.59036000	0.91470300	-1.33129700
O	1.30590900	2.94906400	0.46656400
C	0.92436800	1.84273000	-0.08220100
O	-1.42811800	0.97580900	0.75326100
C	-2.49668300	0.25879800	0.38319100
C	-2.88411100	-0.84844000	1.17855400
C	-3.28119400	0.55721700	-0.75724500
C	-4.01183500	-1.60415400	0.85832500
H	-2.28548700	-1.09024000	2.05280700
C	-4.40077200	-0.21804000	-1.07529000

H	-3.02099500	1.40509100	-1.38279200
C	-4.78025600	-1.30098900	-0.27473500
H	-4.28914200	-2.44185100	1.49394600
H	-4.98588600	0.03538300	-1.95623100
H	-5.65381200	-1.89523600	-0.52572900

Geom 9:
Energy: -765.87642591 Hartrees

C	3.72362500	-1.46464300	-0.13441300
C	2.30350700	-1.67023600	-0.34562800
C	1.41736200	-0.61621400	-0.31784800
C	1.86530700	0.71777000	-0.09891400
C	3.25338900	0.93470600	0.13376500
C	4.15547300	-0.10487200	0.11297400
H	1.96182700	-2.68715100	-0.51555900
H	0.35839600	-0.80710700	-0.45305600
H	3.58237800	1.95074100	0.32137400
H	5.21536800	0.06485900	0.27981700
O	4.54432600	-2.43493400	-0.15602800
C	-0.39085800	1.75950200	-0.58623800
H	-0.92132700	2.69423300	-0.72868200
H	-0.60902100	0.98941000	-1.31917000
O	1.35408700	2.97578200	0.46267700
C	0.93717800	1.88626600	-0.08547200
O	-1.45718600	1.06944600	0.78631500
C	-2.47897600	0.29814700	0.40884300
C	-2.78141300	-0.87247200	1.15114700
C	-3.30392000	0.59875100	-0.70459800
C	-3.86508100	-1.68217900	0.80983100
H	-2.15364700	-1.11918000	2.00350900
C	-4.37669100	-0.22962100	-1.04585900
H	-3.10603600	1.49295800	-1.28794500
C	-4.67179000	-1.37365700	-0.29484500
H	-4.07734400	-2.56673000	1.40601200
H	-4.99301000	0.02822900	-1.90409400
H	-5.51007200	-2.01009000	-0.56238900

Geom 10:
Energy: -765.87685288 Hartrees

C	3.61102000	-1.51668300	-0.13152700
C	2.18131000	-1.67378100	-0.32229800

C	1.33544100	-0.58717400	-0.30082700
C	1.83592100	0.73065600	-0.10615200
C	3.23257800	0.90154800	0.10733700
C	4.09629100	-0.16970000	0.09070800
H	1.80127000	-2.67999700	-0.47277200
H	0.26846900	-0.73961700	-0.42146500
H	3.60028100	1.90749500	0.27713800
H	5.16365800	-0.03692900	0.24193800
O	4.39479900	-2.51517600	-0.14955700
C	-0.37124500	1.85889100	-0.61531400
H	-0.88025900	2.80565200	-0.75079000
H	-0.62597800	1.08222600	-1.32790700
O	1.40490200	3.00465700	0.45059700
C	0.94952000	1.93560500	-0.09882700
O	-1.50372400	1.21039100	0.79308100
C	-2.45795800	0.35983900	0.42329500
C	-2.66887200	-0.83635000	1.15926500
C	-3.30576600	0.59693900	-0.69064600
C	-3.68562700	-1.72723700	0.81352500
H	-2.02475600	-1.03740300	2.01152800
C	-4.30953000	-0.31102600	-1.03679900
H	-3.17411800	1.50703700	-1.26894500
C	-4.51389500	-1.47843400	-0.29030800
H	-3.82819200	-2.62854600	1.40551300
H	-4.94400000	-0.09959000	-1.89462200
H	-5.29931100	-2.17786000	-0.56117300

Geom 11:
Energy: -765.87753698 Hartrees

C	3.52591400	-1.55009900	-0.12987400
C	2.09147000	-1.67108400	-0.31468000
C	1.27531300	-0.56204600	-0.29938300
C	1.81222100	0.74196000	-0.11444100
C	3.21291800	0.87870800	0.09311000
C	4.04833500	-0.21443600	0.08082700
H	1.68466000	-2.66804200	-0.45613900
H	0.20421500	-0.68643200	-0.41567400
H	3.60711300	1.87591500	0.25534400
H	5.11942000	-0.10947100	0.22700900
O	4.28246000	-2.56797200	-0.14359100
C	-0.35409200	1.93417700	-0.64574800
H	-0.85202500	2.88800200	-0.76744500

H	-0.63671300	1.15489000	-1.34365800
O	1.43636900	3.02280200	0.44746500
C	0.95690700	1.97240300	-0.11010500
O	-1.54154900	1.30497700	0.79480700
C	-2.44239700	0.40018600	0.43374000
C	-2.56725400	-0.81972200	1.15295700
C	-3.32113700	0.59713100	-0.66605300
C	-3.53097500	-1.76780800	0.80750200
H	-1.89909000	-0.99246700	1.99301000
C	-4.27094800	-0.36635400	-1.01210000
H	-3.25058300	1.52181500	-1.23256900
C	-4.39008400	-1.55546300	-0.28034900
H	-3.60824200	-2.68515900	1.38699400
H	-4.93002100	-0.18382300	-1.85801700
H	-5.13410700	-2.29900500	-0.55071600

Geom 12:
Energy: -765.87835337 Hartrees

C	3.48734800	-1.56601500	-0.12931900
C	2.05012700	-1.66881400	-0.30607000
C	1.24984700	-0.54838300	-0.29450100
C	1.80630600	0.74808400	-0.11876700
C	3.20930200	0.86810900	0.08035800
C	4.02987700	-0.23591600	0.06989200
H	1.62915400	-2.66105900	-0.43864800
H	0.17646500	-0.65780000	-0.40459600
H	3.61765600	1.86092400	0.23469300
H	5.10315000	-0.14517900	0.20897400
O	4.22956400	-2.59328300	-0.14045600
C	-0.33410600	1.97433900	-0.66907300
H	-0.83376000	2.92870300	-0.77452800
H	-0.63289600	1.19156400	-1.35527900
O	1.45470100	3.02890600	0.45380200
C	0.96654300	1.99140100	-0.11406000
O	-1.56364300	1.33973200	0.80271500
C	-2.43895200	0.41516200	0.44244700
C	-2.51765900	-0.82309000	1.13948600
C	-3.34067500	0.60404800	-0.64201100
C	-3.45803800	-1.79268500	0.79001800
H	-1.83267500	-0.99144300	1.96690100
C	-4.26684600	-0.38004900	-0.99205000
H	-3.30309100	1.54038100	-1.19271200
C	-4.33969400	-1.58586500	-0.28088900

H	-3.49997600	-2.72256600	1.35304700
H	-4.94362900	-0.20229100	-1.82496800
H	-5.06565000	-2.34604500	-0.55412900

Geom 13:
Energy: -765.87921030 Hartrees

C	3.46716400	-1.57567700	-0.12839500
C	2.02936400	-1.66639600	-0.30921500
C	1.23917000	-0.53899300	-0.30134800
C	1.80667900	0.75194900	-0.12294800
C	3.20975100	0.86081800	0.07971600
C	4.02104400	-0.24984300	0.07137900
H	1.60031300	-2.65510600	-0.44208500
H	0.16520700	-0.63865200	-0.41475700
H	3.62603600	1.85021600	0.23507400
H	5.09473400	-0.16842200	0.21269500
O	4.20042400	-2.60856400	-0.13709500
C	-0.31300600	2.00126500	-0.69378300
H	-0.81758200	2.95418200	-0.78468700
H	-0.62383200	1.21419200	-1.36876200
O	1.46736300	3.03135000	0.45965800
C	0.97698100	2.00337400	-0.11841000
O	-1.58008000	1.35600300	0.81064900
C	-2.44035600	0.42236400	0.45023900
C	-2.48998300	-0.82937300	1.12854400
C	-3.36028800	0.61067300	-0.62085700
C	-3.41798400	-1.80931700	0.77573100
H	-1.79225800	-0.99862200	1.94510300
C	-4.27399600	-0.38318800	-0.97402800
H	-3.34373400	1.55558000	-1.15799700
C	-4.31707900	-1.60117500	-0.28050400
H	-3.43723300	-2.74835000	1.32469900
H	-4.96444500	-0.20485400	-1.79557500
H	-5.03363300	-2.36937000	-0.55613100

Geom 14:
Energy: -765.88005752 Hartrees

C	3.45518900	-1.58038700	-0.12704000
C	2.01878200	-1.66222000	-0.32393100
C	1.23525800	-0.53033600	-0.32046100

C	1.80801100	0.75611100	-0.12849000
C	3.20919000	0.85659400	0.08952200
C	4.01449000	-0.25828400	0.08447800
H	1.58562100	-2.64790200	-0.46553600
H	0.16217000	-0.62350100	-0.44646000
H	3.62911400	1.84299600	0.25406000
H	5.08706800	-0.18358100	0.23730900
O	4.18271100	-2.61677800	-0.13264300
C	-0.29397100	2.02192400	-0.72148300
H	-0.80430200	2.97256300	-0.80083400
H	-0.61544200	1.22914100	-1.38390100
O	1.47479100	3.03462900	0.46034100
C	0.98553400	2.01313600	-0.12587700
O	-1.59578500	1.36615800	0.81796800
C	-2.44392700	0.42575600	0.45853700
C	-2.45696400	-0.84322100	1.10894800
C	-3.39245000	0.62015200	-0.58818800
C	-3.37519400	-1.83129900	0.75455700
H	-1.73845000	-1.01806900	1.90603300
C	-4.29668700	-0.38112000	-0.94256000
H	-3.40291100	1.57681000	-1.10443200
C	-4.30225800	-1.61525500	-0.27586800
H	-3.36581900	-2.78279200	1.28191500
H	-5.00916700	-0.19733000	-1.74385600
H	-5.01163400	-2.38971800	-0.55248800

Geom 15:
Energy: -765.88087636 Hartrees

C	3.43678600	-1.58781700	-0.12513400
C	2.00389500	-1.65686600	-0.35105200
C	1.22905100	-0.51918600	-0.35284700
C	1.80674000	0.76089300	-0.13546300
C	3.20400900	0.84883600	0.11048900
C	4.00131100	-0.27168300	0.11001000
H	1.56621700	-2.63783800	-0.51034100
H	0.15825600	-0.60389600	-0.50150900
H	3.62758500	1.83056900	0.29284400
H	5.07123300	-0.20627400	0.28420500
O	4.15685400	-2.62907400	-0.12679900
C	-0.27379000	2.04705800	-0.75325000
H	-0.78692500	2.99683400	-0.82256700
H	-0.60677200	1.24999700	-1.40405800
O	1.48306100	3.03961700	0.45909500

C	0.99444300	2.02477200	-0.13569900
O	-1.61308700	1.38375500	0.82011600
C	-2.44573400	0.43257500	0.46515500
C	-2.42184400	-0.84741900	1.09666500
C	-3.41884200	0.62247900	-0.56167900
C	-3.32679200	-1.84785200	0.74464400
H	-1.68496600	-1.01951200	1.87734500
C	-4.31008700	-0.39056100	-0.91292500
H	-3.45599100	1.58596200	-1.06387100
C	-4.27826400	-1.63438300	-0.26424300
H	-3.28899600	-2.80691800	1.25672500
H	-5.04174500	-0.20990200	-1.69744700
H	-4.97781400	-2.41848200	-0.53864400

Geom 16:
Energy: -765.88166393 Hartrees

C	3.36308900	-1.61765500	-0.12526100
C	1.94845700	-1.64240800	-0.45229600
C	1.20055900	-0.48706500	-0.46297300
C	1.78711100	0.76983500	-0.15306300
C	3.16622600	0.81365900	0.18826400
C	3.93750200	-0.32488300	0.19891100
H	1.50121600	-2.60533400	-0.68023400
H	0.14207900	-0.54344100	-0.69049400
H	3.59689800	1.77790600	0.43565300
H	4.99395500	-0.29134000	0.44840900
O	4.05895400	-2.67521800	-0.11801600
C	-0.24365700	2.11476100	-0.80537300
H	-0.74448200	3.07213200	-0.85815700
H	-0.59770200	1.32639900	-1.45481200
O	1.50239400	3.04961800	0.46197200
C	1.00664000	2.05307300	-0.15454700
O	-1.62907000	1.44513600	0.79491000
C	-2.42611300	0.46062900	0.46497800
C	-2.36949900	-0.79968500	1.13675100
C	-3.39643400	0.58928600	-0.57633500
C	-3.23972400	-1.83689200	0.80782200
H	-1.63382100	-0.92490300	1.92743100
C	-4.25265200	-0.46035800	-0.90289600
H	-3.45635100	1.53550500	-1.10815300
C	-4.18799700	-1.68250600	-0.21545700
H	-3.17810500	-2.77875700	1.34851500

H	-4.98236100	-0.32748300	-1.69859500
H	-4.86060800	-2.49572900	-0.47165400

Geom 17:
Energy: -765.88248976 Hartrees

C	3.30661400	-1.63554200	-0.12987400
C	1.94314200	-1.60577600	-0.62704700
C	1.21688500	-0.43688300	-0.64842100
C	1.77272900	0.78541300	-0.18140900
C	3.10287500	0.77473600	0.31964900
C	3.85213400	-0.37831700	0.34669000
H	1.51352400	-2.54043400	-0.97528100
H	0.19530500	-0.46107200	-1.00965500
H	3.51429000	1.71118900	0.68058800
H	4.87079400	-0.38184800	0.72363600
O	3.98291800	-2.70635800	-0.10941200
C	-0.21699600	2.17466400	-0.85893700
H	-0.71940100	3.13280000	-0.87793800
H	-0.59029400	1.39850500	-1.51124000
O	1.50925300	3.06288800	0.46047000
C	1.01826300	2.08098100	-0.18022200
O	-1.57472900	1.41980200	0.79633400
C	-2.38042400	0.44588000	0.48039700
C	-2.30587800	-0.82591900	1.13464300
C	-3.38491100	0.59284700	-0.52948700
C	-3.18936900	-1.85400800	0.81990100
H	-1.54391000	-0.96282700	1.89768100
C	-4.25484800	-0.44808000	-0.83988900
H	-3.45619400	1.54661000	-1.04571400
C	-4.17072300	-1.67975700	-0.16967700
H	-3.11500300	-2.80424300	1.34358000
H	-5.01076700	-0.30398700	-1.60838200
H	-4.85483300	-2.48678900	-0.41429800

Geom 18:
Energy: -765.88437447 Hartrees

C	3.16117800	-1.68217100	-0.14444700
C	1.92506700	-1.52430000	-0.88616700
C	1.25284000	-0.32299400	-0.91328000
C	1.73705400	0.81491100	-0.21143900

C	2.94868400	0.67929200	0.51974900
C	3.64014100	-0.50941300	0.56143800
H	1.54395800	-2.38977500	-1.42065700
H	0.32991800	-0.25924300	-1.47808900
H	3.31597100	1.54992500	1.05262900
H	4.56436500	-0.60326000	1.12492400
O	3.78686500	-2.78535300	-0.11367600
C	-0.17470300	2.29504400	-0.91042600
H	-0.66100400	3.26186100	-0.88304900
H	-0.57891200	1.54784400	-1.57711200
O	1.53548000	3.08641200	0.48134100
C	1.04011600	2.13530300	-0.19902500
O	-1.50875900	1.43094200	0.77963600
C	-2.29925500	0.44728800	0.49146800
C	-2.20028600	-0.81512800	1.16982300
C	-3.31705200	0.56637700	-0.51475600
C	-3.06905500	-1.85851900	0.87713400
H	-1.42956400	-0.92613500	1.92768600
C	-4.17298900	-0.48996200	-0.79851900
H	-3.40426400	1.51168000	-1.04311900
C	-4.06111200	-1.70998000	-0.10798900
H	-2.97873400	-2.80056600	1.41206800
H	-4.93919500	-0.37224400	-1.56067600
H	-4.73500000	-2.53058800	-0.33439200

Geom 19:
Energy: -765.88454213 Hartrees

C	3.08624000	-1.71964000	-0.15468700
C	1.89474800	-1.50045300	-0.94962200
C	1.25730800	-0.27943800	-0.97140100
C	1.73429100	0.82398100	-0.21206500
C	2.90393800	0.62781600	0.57167400
C	3.55888200	-0.58209500	0.60946900
H	1.51629600	-2.33597100	-1.53199300
H	0.36736100	-0.17358800	-1.58147200
H	3.27014400	1.46920100	1.15076400
H	4.45062000	-0.71803300	1.21562300
O	3.68030700	-2.84233200	-0.12773200
C	-0.12064300	2.36138000	-0.93043100
H	-0.59296200	3.33468400	-0.88344500
H	-0.53919300	1.63031700	-1.60619900
O	1.57351400	3.09095400	0.51085100

C	1.07564500	2.15804400	-0.19183300
O	-1.50140100	1.45092000	0.76714400
C	-2.27878700	0.46187100	0.49038100
C	-2.17809600	-0.79004100	1.19456500
C	-3.28720500	0.55823900	-0.53227500
C	-3.03343000	-1.84329400	0.90742500
H	-1.41552900	-0.87990300	1.96297600
C	-4.13029200	-0.50801800	-0.80711000
H	-3.37303000	1.49465000	-1.07590200
C	-4.01441100	-1.71570100	-0.09335700
H	-2.94439200	-2.77671100	1.45684900
H	-4.88896600	-0.41159100	-1.57926600
H	-4.67882900	-2.54529500	-0.31444300

Geom 20:
Energy: -765.88558920 Hartrees

C	3.06288900	-1.74267700	-0.15876300
C	1.88622600	-1.49597300	-0.96577600
C	1.26661000	-0.26502600	-0.98413000
C	1.74766100	0.82535200	-0.20862400
C	2.90316100	0.60145400	0.58827600
C	3.53967800	-0.61893000	0.62205900
H	1.50209200	-2.31899800	-1.56245500
H	0.38689200	-0.14176700	-1.60610700
H	3.27544600	1.43035200	1.18174500
H	4.42131900	-0.77238400	1.23911600
O	3.64165800	-2.87519100	-0.13524400
C	-0.07223900	2.39450000	-0.94345400
H	-0.53561300	3.37187200	-0.88794500
H	-0.49839500	1.67150000	-1.62335600
O	1.60519800	3.08889400	0.53208000
C	1.10977600	2.16491400	-0.18392700
O	-1.51430100	1.45884800	0.75998700
C	-2.28787400	0.47193900	0.48853000
C	-2.19903800	-0.77227000	1.21326300
C	-3.28304900	0.55810900	-0.55178200
C	-3.05007300	-1.82676700	0.92595900
H	-1.44764500	-0.85108300	1.99352100
C	-4.12222600	-0.50960000	-0.82430700
H	-3.35773400	1.48819800	-1.10737400
C	-4.01598700	-1.70829300	-0.09198700
H	-2.97205500	-2.75409600	1.48674700

H	-4.86994500	-0.42444100	-1.60803300
H	-4.67790200	-2.53995700	-0.31245600

Geom 21:
Energy: -765.88656523 Hartrees

C	3.04603200	-1.76491700	-0.16105000
C	1.87745700	-1.49671300	-0.97152100
C	1.27428000	-0.25700700	-0.98725100
C	1.76484400	0.82430300	-0.20494600
C	2.91278300	0.57880600	0.59627500
C	3.53260200	-0.65074200	0.62659700
H	1.48382900	-2.31078000	-1.57458500
H	0.39939200	-0.12028200	-1.61358300
H	3.29473700	1.39868500	1.19645300
H	4.40936800	-0.81772400	1.24741400
O	3.61033900	-2.90621600	-0.14007000
C	-0.02331200	2.42231800	-0.95368000
H	-0.47678200	3.40420300	-0.89278100
H	-0.45704200	1.70654300	-1.63667800
O	1.64036700	3.08497900	0.55002400
C	1.14552000	2.16908100	-0.17675100
O	-1.53486400	1.47098100	0.75259500
C	-2.30401900	0.48454200	0.48553700
C	-2.22800400	-0.75033000	1.23174600
C	-3.28367000	0.55783500	-0.57346600
C	-3.07398500	-1.80724000	0.94473300
H	-1.48937800	-0.81680700	2.02504600
C	-4.11797300	-0.51250100	-0.84390600
H	-3.34710200	1.48046000	-1.14249900
C	-4.02287800	-1.70075500	-0.09163500
H	-3.00729900	-2.72723500	1.51854100
H	-4.85300600	-0.43993400	-1.64053400
H	-4.68152800	-2.53516500	-0.31127500

Geom 22:
Energy: -765.88745030 Hartrees

C	2.97500500	-1.80893400	-0.16680700
C	1.83046100	-1.49407300	-0.99368900
C	1.26527400	-0.23612600	-1.00468800

C	1.77371300	0.82128700	-0.20152700
C	2.89918300	0.52999300	0.61592200
C	3.48051900	-0.71871100	0.64159500
H	1.42178400	-2.28763400	-1.61400000
H	0.40627900	-0.06630200	-1.64503200
H	3.29653800	1.33009400	1.23285500
H	4.34092200	-0.91879100	1.27562100
O	3.50376300	-2.96827400	-0.14906600
C	0.04855800	2.48007900	-0.96488700
H	-0.37905800	3.47329800	-0.89715800
H	-0.39982800	1.78270000	-1.65759200
O	1.70096400	3.07651800	0.57754300
C	1.19499500	2.18140100	-0.16737500
O	-1.56423500	1.52764700	0.72107900
C	-2.30881500	0.52171900	0.47150800
C	-2.23169100	-0.68522900	1.26499700
C	-3.26260500	0.54096900	-0.61542000
C	-3.05130900	-1.76562000	0.99400600
H	-1.51269900	-0.70933800	2.07837000
C	-4.07050500	-0.55246700	-0.86824200
H	-3.32556500	1.44187800	-1.21822400
C	-3.97424800	-1.71127100	-0.07039400
H	-2.98527100	-2.66395500	1.60100000
H	-4.78545800	-0.52273600	-1.68545100
H	-4.61278800	-2.56444300	-0.27683400

Geom 23:
Energy: -765.88825040 Hartrees

C	2.88540900	-1.85358000	-0.17483000
C	1.79299100	-1.47853300	-1.04527300
C	1.27097300	-0.20176500	-1.04985100
C	1.77661400	0.81862800	-0.19845000
C	2.85162200	0.46793400	0.66232800
C	3.38772000	-0.80116800	0.68369800
H	1.38791100	-2.24168700	-1.70502500
H	0.45062200	0.01293700	-1.72661100
H	3.24634900	1.23813500	1.31796900
H	4.20882800	-1.04650100	1.35310000
O	3.37345200	-3.03131200	-0.16203600
C	0.12717400	2.54462900	-0.97855100
H	-0.27178500	3.54930600	-0.90234700
H	-0.33532200	1.86928300	-1.68388100

O	1.76035800	3.06489600	0.61058400
C	1.24466100	2.19581600	-0.15824500
O	-1.59190200	1.59321800	0.67819600
C	-2.30538700	0.56203000	0.45237700
C	-2.20863600	-0.61653100	1.28745500
C	-3.24402700	0.52121600	-0.64858300
C	-2.99576500	-1.72565100	1.04067100
H	-1.50094200	-0.59463900	2.11067000
C	-4.01950400	-0.60015500	-0.87580400
H	-3.32024300	1.40021200	-1.28141800
C	-3.90443300	-1.72912600	-0.03791700
H	-2.91610200	-2.60216000	1.67707800
H	-4.72312900	-0.61686200	-1.70303700
H	-4.51793100	-2.60491800	-0.22460200

Geom 24:
Energy: -765.88896209 Hartrees

C	2.90713200	-1.85380000	-0.16883800
C	1.80986500	-1.48293200	-1.03439800
C	1.28653300	-0.20649000	-1.04204400
C	1.79594600	0.81897100	-0.19877300
C	2.87579700	0.47219200	0.65741400
C	3.41292300	-0.79662200	0.68143600
H	1.40119900	-2.24904100	-1.68861200
H	0.46250000	0.00390200	-1.71587200
H	3.27412600	1.24525400	1.30759800
H	4.23803900	-1.03766500	1.34759300
O	3.39644800	-3.03156500	-0.15305700
C	0.14364300	2.54120900	-0.98195300
H	-0.25298000	3.54725700	-0.91061800
H	-0.32687700	1.86032100	-1.67675900
O	1.78067300	3.06933800	0.60000400
C	1.26381300	2.19490600	-0.16234300
O	-1.65542500	1.61376600	0.68175600
C	-2.35009200	0.57245500	0.45460300
C	-2.23626900	-0.60511100	1.29089000
C	-3.28408900	0.51622400	-0.65119000
C	-3.00163800	-1.72748500	1.03931800
H	-1.53299000	-0.57033000	2.11736600
C	-4.03772900	-0.61832500	-0.88243300
H	-3.37226900	1.39448500	-1.28341900
C	-3.90512200	-1.74565200	-0.04412900

H	-2.90971700	-2.60335600	1.67479800
H	-4.73724600	-0.64804500	-1.71267000
H	-4.50163200	-2.63233000	-0.23438400

Geom 25:
Energy: -765.88959630 Hartrees

C	2.93068900	-1.85145200	-0.16404500
C	1.83250100	-1.48477500	-1.02984600
C	1.30599200	-0.20954500	-1.04044300
C	1.81318700	0.81972900	-0.20025100
C	2.89433500	0.47705400	0.65594600
C	3.43420500	-0.79063900	0.68287000
H	1.42522000	-2.25308200	-1.68243200
H	0.48167500	-0.00292900	-1.71521800
H	3.29176300	1.25237000	1.30406100
H	4.26021900	-1.02776400	1.34941300
O	3.42277500	-3.02839100	-0.14514400
C	0.15522000	2.53542300	-0.98596600
H	-0.24043200	3.54232600	-0.91986000
H	-0.32312700	1.84772500	-1.66881200
O	1.79696400	3.07439800	0.58695900
C	1.27943600	2.19411800	-0.16827900
O	-1.68860900	1.60898400	0.70850600
C	-2.38031500	0.57028900	0.46790500
C	-2.25836900	-0.62116600	1.28443300
C	-3.31934700	0.52938500	-0.63533500
C	-3.01950800	-1.74205800	1.01630600
H	-1.55226100	-0.59692900	2.10881700
C	-4.06857400	-0.60409800	-0.88298400
H	-3.41328500	1.41812500	-1.25183200
C	-3.92705200	-1.74508200	-0.06433300
H	-2.92175000	-2.62854500	1.63589000
H	-4.77126400	-0.62322800	-1.71077800
H	-4.52020500	-2.63109700	-0.26767100

Geom 26:
Energy: -765.89015720 Hartrees

C	2.94985800	-1.85303900	-0.15968000

C	1.84684100	-1.48962600	-1.02042900
C	1.32036600	-0.21434200	-1.03366200
C	1.83241300	0.81900100	-0.20119000
C	2.91847500	0.47944500	0.65002900
C	3.45822600	-0.78831500	0.67928300
H	1.43540200	-2.26049300	-1.66742700
H	0.49234800	-0.01083200	-1.70493600
H	3.32023700	1.25731500	1.29244600
H	4.28818200	-1.02231600	1.34208900
O	3.44205100	-3.03016800	-0.13830700
C	0.17190900	2.53183800	-0.98762300
H	-0.21988700	3.54072700	-0.92723700
H	-0.31552200	1.83893500	-1.65883600
O	1.82193300	3.07815200	0.57381300
C	1.30033600	2.19325900	-0.17328700
O	-1.72022600	1.60579900	0.73313700
C	-2.41004000	0.57017600	0.47975400
C	-2.28182900	-0.63390600	1.27767000
C	-3.35374400	0.54433100	-0.62080600
C	-3.04043500	-1.75235600	0.99438600
H	-1.57299700	-0.62014800	2.09991200
C	-4.10025700	-0.58710900	-0.88354600
H	-3.45215000	1.44260800	-1.22255700
C	-3.95185700	-1.74051200	-0.08328300
H	-2.93822400	-2.64843800	1.59918600
H	-4.80598700	-0.59568100	-1.70886800
H	-4.54303800	-2.62500200	-0.29860700

Geom 27:
Energy: -765.89005537 Hartrees

C	2.93481100	-1.87734600	-0.16059900
C	1.85134400	-1.48962800	-1.03814100
C	1.34257300	-0.20562500	-1.04942400
C	1.85386100	0.81459300	-0.19956200
C	2.92038800	0.45256300	0.66742000
C	3.44236900	-0.82403300	0.69624900
H	1.44071400	-2.24893900	-1.69942300
H	0.53006500	0.01526000	-1.73437500
H	3.32200800	1.21949800	1.32311600
H	4.25693800	-1.07439800	1.37224300
O	3.41366000	-3.06994000	-0.13983200
C	0.22037100	2.55365200	-1.00107500

H	-0.15887300	3.56759500	-0.94360500
H	-0.27232800	1.86631600	-1.67480600
O	1.87165000	3.08737700	0.59503400
C	1.34023200	2.19867000	-0.17102900
O	-1.73486800	1.62501000	0.72748100
C	-2.42849600	0.58259000	0.47559000
C	-2.30953100	-0.61755000	1.28521500
C	-3.36558800	0.54857700	-0.63354700
C	-3.06881900	-1.73631000	1.00506500
H	-1.60711000	-0.59878200	2.11283600
C	-4.11241300	-0.58365600	-0.89205100
H	-3.45729800	1.44181600	-1.24376000
C	-3.97238100	-1.73085200	-0.08019600
H	-2.97385300	-2.62782900	1.61779300
H	-4.81198400	-0.59826400	-1.72255200
H	-4.56413800	-2.61572800	-0.29241300

Geom 28:
Energy: -765.891166206 Hartrees

C	3.01846200	-1.88999000	-0.15853900
C	1.95137700	-1.48086600	-1.04269500
C	1.44420700	-0.19753300	-1.03256500
C	1.94235100	0.80155400	-0.15047300
C	2.99133300	0.41567600	0.72695900
C	3.51142400	-0.86093800	0.73205000
H	1.55013900	-2.22380300	-1.72790100
H	0.64216600	0.03936300	-1.72450900
H	3.38244900	1.16500400	1.40895800
H	4.31460700	-1.12866700	1.41501400
O	3.49418600	-3.07495200	-0.16024800
C	0.36372700	2.57659000	-0.96798000
H	-0.00982300	3.59134600	-0.89241100
H	-0.09981100	1.91931300	-1.68994000
O	1.92051500	3.02897400	0.71351400
C	1.43233300	2.18139900	-0.09756400
O	-2.04875100	1.79600800	0.26627500
C	-2.63792900	0.67448600	0.24083900
C	-2.50833300	-0.27048000	1.33562200
C	-3.46503700	0.28359400	-0.88657300
C	-3.15641500	-1.48775900	1.29526300
H	-1.88816700	0.01760400	2.17877300
C	-4.10231500	-0.94001100	-0.90179300

H	-3.56263100	0.98731700	-1.70746300
C	-3.95526600	-1.83282600	0.18273300
H	-3.05501900	-2.18818000	2.11868800
H	-4.72034800	-1.22380300	-1.74822100
H	-4.46067300	-2.79312000	0.16098700

Geom 29:
Energy: -765.89156951 Hartrees

C	2.96938900	-1.91692100	-0.15541700
C	1.90835300	-1.49047200	-1.03873800
C	1.42657400	-0.19742500	-1.03275700
C	1.94637500	0.79537300	-0.15604700
C	2.98995600	0.39257900	0.72036100
C	3.48454200	-0.89403800	0.72981000
H	1.49095900	-2.22813200	-1.71998500
H	0.62810100	0.05236600	-1.72428800
H	3.39767000	1.13683500	1.39820700
H	4.28370300	-1.17465100	1.41231900
O	3.42190000	-3.11090100	-0.15352300
C	0.39826500	2.59652800	-0.97482800
H	0.04693200	3.61970100	-0.90426200
H	-0.08584500	1.94307000	-1.68684200
O	1.97376700	3.02776200	0.69478700
C	1.46434700	2.18517000	-0.10825600
O	-2.02678600	1.80324100	0.33935400
C	-2.62131500	0.68622100	0.27648000
C	-2.51529800	-0.28568800	1.35006600
C	-3.43161900	0.32767500	-0.87374800
C	-3.16969400	-1.49758000	1.26966000
H	-1.90766100	-0.02156000	2.21001000
C	-4.07547300	-0.89129600	-0.92908200
H	-3.51130100	1.05152200	-1.67891900
C	-3.95176100	-1.81072800	0.13597700
H	-3.08621100	-2.21828700	2.07745100
H	-4.68089500	-1.15101800	-1.79217400
H	-4.46234400	-2.76704600	0.08265000

Geom 30:

Energy: -765.89192519 Hartrees

C	2.96029200	-1.92820700	-0.15352000
C	1.90200700	-1.49447500	-1.03661000
C	1.43074600	-0.19759500	-1.03231200
C	1.95921500	0.79242100	-0.15751700
C	3.00015600	0.38241100	0.71873100
C	3.48423300	-0.90813400	0.72984400
H	1.47821300	-2.22971500	-1.71652700
H	0.63399300	0.05754700	-1.72387400
H	3.41442200	1.12435500	1.39513500
H	4.28154600	-1.19405600	1.41232100
O	3.40333100	-3.12570200	-0.15032800
C	0.42458900	2.60446700	-0.97740700
H	0.08406900	3.63166500	-0.91059600
H	-0.06992500	1.95193400	-1.68323900
O	2.00808400	3.02687700	0.68697900
C	1.48945300	2.18623800	-0.11212600
O	-2.04317500	1.81070100	0.36678000
C	-2.63485900	0.69337300	0.28957100
C	-2.53079500	-0.28980200	1.35321500
C	-3.44018300	0.34564200	-0.86761500
C	-3.18245400	-1.50196000	1.25734500
H	-1.92683100	-0.03361300	2.21813200
C	-4.08130900	-0.87389800	-0.93839400
H	-3.51819400	1.07802100	-1.66518900
C	-3.95966300	-1.80436200	0.11734600
H	-3.10063200	-2.23120000	2.05759800
H	-4.68301400	-1.12561800	-1.80642700
H	-4.46813400	-2.76105200	0.05191000

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