Supporting Information

Visible-Light-Induced Upcycling of Perchloroethylene into Trichloroacetamides Using Chlorine Dioxide

Shohei Ohno,[a] Genta Taniguchi,[a] Minami Fukuhara,[a] Yuki Itabashi,[b] Tsuyoshi Inoue,[a,b] Kei Ohkubo,[b,c] and Haruyasu Asahara[a,b]*

[a] Graduate School of Pharmaceutical Sciences, The University of Osaka, 1-6 Yamadaoka, Suita, Osaka 565-0871, Japan

[b] Institute for Open and Transdisciplinary Research Initiatives (OTRI), The University of Osaka, 1-6 Yamadaoka, Suita, Osaka 565-0871, Japan

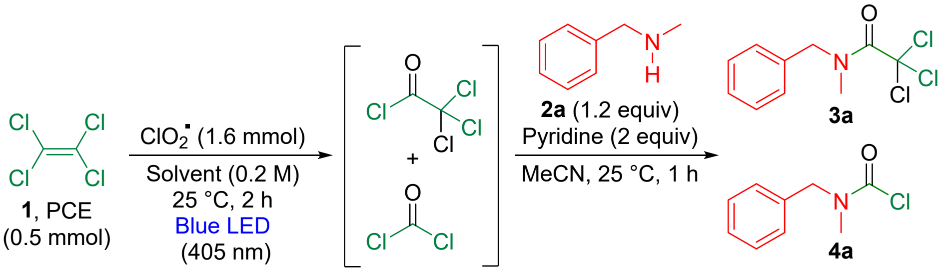
[c] Organization for Carbon Neutrality Collaboration (OCNC), The University of Osaka, 1-6 Yamadaoka, Suita, Osaka 565-0871, Japan

* Corresponding author: asahara@phs.osaka-u.ac.jp

Table of Contents

1. Additional screening of solvents (Table S1) and ESR spectra (Fig. S1)

Table S1 A screening of green solvents and other electron-deficient aromatic solvents



Entry	Solvent	Yield (%)$^{(a)}$	
		3a	**4a**$^{(b)}$
1	Propylene carbonate	3	0
2	*o*-Dichlorobenzene	31	3
3	Benzonitrile	13	1

(a) NMR yield based on PCE (b) Yield was calculated based on two molecules of phosgene per **1**

In this reaction system, highly reactive chlorine radicals are generated under oxidative conditions. As a result, solvents susceptible to radical oxidation, such as tetrahydrofuran, 2-methyltetrahydrofuran, and other ether-type solvents, are unsuitable because they undergo rapid solvent degradation under the reaction conditions. In addition, the key reactive intermediates in this system are acyl chlorides formed in situ. Therefore, nucleophilic solvents such as ethanol are incompatible, as they readily react with these intermediates, preventing the desired amide formation. We examined several alternative solvents (**Table S1**), including propylene carbonates, and other electron-deficient aromatic solvents. When propylene carbonate was used as a representative green solvent, the desired product was obtained in only 3% yield (entry 1). *o*-Dichlorobenzene and benzonitrile were also evaluated as oxidation-resistant aromatic solvents; however, these solvents afforded only moderate efficiencies, giving the desired products in 31% and 13% yields, respectively (entries 2-3). Based on the overall evaluation of reaction efficiency, solvent compatibility, and substrate scope, PCBTF was selected as the most suitable solvent for the present study.

Regarding safety considerations, the reactions were conducted under closed conditions, and PCBTF, owing to its high boiling point, can be readily recovered and recycled after the reaction. From the viewpoint of solvent reuse and containment, this feature represents a practical advantage of PCBTF in the current system. However, it should be noted that the use of PCBTF does not eliminate safety concerns. Appropriate precautions, including adequate ventilation and standard laboratory safety measures, remain necessary when handling this solvent.

2. ESR spectra (Fig. S1)

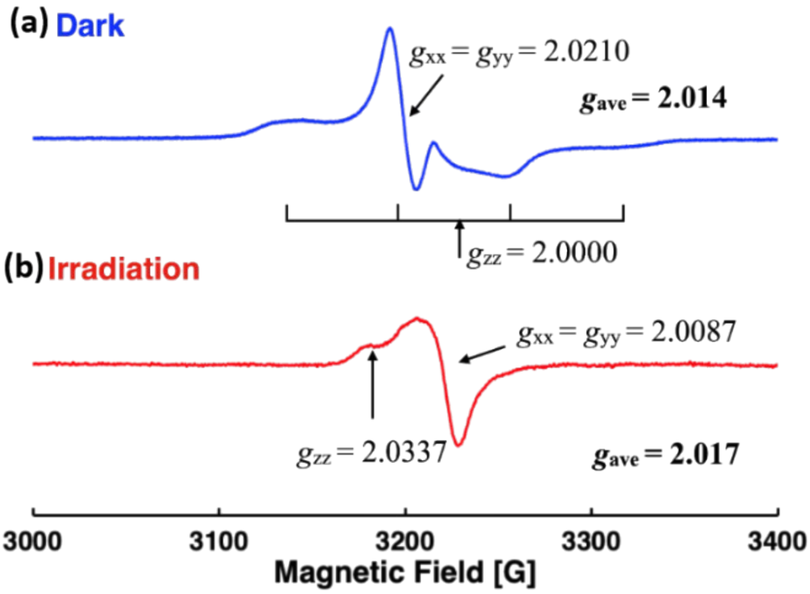
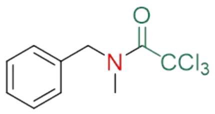


Fig. S1 ESR spectra of PCE solution containing $ClO_2^{\bullet}$ (a) before and (b) after LED irradiation (λ = 405 nm). The spectra were observed at −120 ˚C by rapid freezing under photoirradiation.

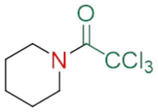
3. Preparation of compounds 3a-j

Experimental procedure

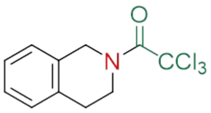
An aqueous chlorine dioxide solution was prepared by dissolving sodium chlorite ($NaClO_2$, 200 mg, 2.0 mmol (1.6 mmol of $ClO_2^{\bullet}$))[S1] and 35% hydrochloric acid (100 µL) in purified water (5 mL), and placed in chamber A. Chamber B was charged with 1-chloro-4-(trifluoromethyl)benzene (PCBTF, 1 mL) and tetrachloroethylene (51.5 µL, 0.5 mmol). After sealing, the entire H-shaped tube was irradiated with 405 nm LED light (90 mW cm^{-2}) for 2 h at room temperature. Subsequently, a solution of amine (0.6 mmol) and pyridine (80.8 µL, 1.0 mmol) in MeCN (1 mL) was added to chamber B, and the mixture was stirred for 1 h. The reaction was conducted in a sealed system. After completion, the reaction vessel was carefully opened in a well-ventilated fume hood, and the reaction mixture was cautiously quenched with saturated aqueous $NaHCO_3$ under stirring. Particular care was taken to ensure complete neutralization of residual oxidizing species prior to further workup. The mixture was then extracted with chloroform, and the organic layer was dried over anhydrous magnesium sulfate ($MgSO_4$). After evaporation of the solvent under reduced pressure, the residue was purified by column chromatography to afford the desired product.



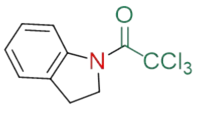
N-Benzyl-*N*-methyl-2,2,2-trichloroacetamide (**3a**): Colorless oil. IR (KBr): 3031, 2929, 1671, 1390, 1250, 1110, 804, 668 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$, 50 °C): δ 7.37–7.25 (m, 5H), 4.75 (s, 2H), 3.19 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 50 °C): δ 161.0, 135.6, 128.8, 127.9, 127.0, 93.3, 54.9, 37.8. HRMS (ESI) m/z: [M + Na]$^{+}$ calcd. for $C_{19}H_{10}Cl_3NNaO$: 287.9720, found: 287.9723.



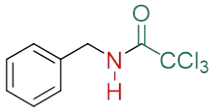
N-Trichloracetyl-piperidine (**3b**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.81–3.68 (br, 4H), 1.69 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.1, 93.4, 49.4, 47.3, 47.0, 25.6, 24.1. The obtained NMR spectra are consistent with the reported data.[S2]



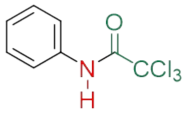
2-Trichloroacetyl-1,2,3,4-tetrahydroquinoline (**3c**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.25–7.15 (m, 4H), 5.02–4.83 (br, 2H), 4.11–3.92 (br, 2H), 2.97 (t, *J* = 5.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.4, 132.1, 131.9, 128.5, 127.0, 126.6, 126.3, 93.0, 47.7, 45.7, 28.6. The obtained NMR spectra are consistent with the reported data. [S3]



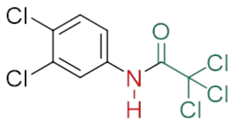
1-(Trichloroacetyl)indoline (**3d**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.20 (d, *J* = 8.3 Hz, 1H), 7.30–7.26 (m, 2H), 7.15 (dd, *J* = 8.3, 1.0 Hz, 1H), 4.56 (t, *J* = 8.1 Hz, 2H), 3.23 (t, *J* = 8.1 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.8, 143.1, 131.7, 127.8, 125.5, 124.7, 118.6, 93.8, 51.2, 29.2. The obtained NMR spectra are consistent with the reported data. [S4]



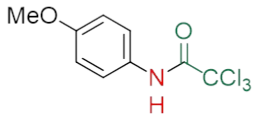
N-Benzyl-2,2,2-trichloroacetamide (**3e**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41–7.31 (m, 5H), 6.49 (br, 1H), 4.56 (d, *J* = 5.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.9, 136.2, 129.0, 128.2, 127.8, 92.5, 45.4. The obtained NMR spectra are consistent with the reported data. [S2]



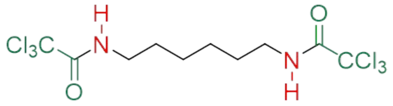
Trichloroacetanilide (**3f**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.33 (br, 1H), 7.58 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.23 (t, *J* = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.2, 135.9, 129.6, 126.0, 120.3, 92.8. The obtained NMR spectra are consistent with the reported data. [S2]



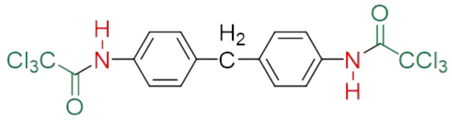
2,2,2-Trichloro-*N*-(3,4-dichlorophenyl)acetamide (**3g**): Colorless oil. IR (KBr): 3259, 3095, 3020, 1682, 1511, 1093, 808, 656 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.30 (br, 1H), 7.80 (d, *J* = 2.3 Hz 1H), 7.46 (d, *J* = 8.7 Hz, 1H), 7.41 (dd, *J* = 8.7, 2.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.3, 135.3, 133.3, 130.8, 129.6, 122.2, 119.6, 92.3. HRMS (ESI) m/z: $[M + Na]^+$ calcd. for $C_8H_4Cl_5NNaO$: 327.8628, found: 327.8630.



2,2,2-Trichloro-*N*-(4-methoxyphenyl)acetamide (**3h**): White solid. mp 117.1-117.9 ºC. IR (KBr): 3297, 2936, 1685, 1492, 1226, 1033, 808, 618 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.27 (br, 1H), 7.51 (d, *J* = 7.8 Hz, 2H), 6.95 (d, *J* = 7.8 Hz, 2H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.2, 157.6, 128.8, 122.1, 114.4, 92.9, 55.5. HRMS (ESI) m/z: $[M + Na]^+$ calcd. for $C_9H_8Cl_3NNaO_2$: 289.9513, found: 289.9512.



2,2,2-Trichloro-*N*-[6-[(2,2,2-trichloroacetyl)amino]hexyl] acetamide (**3i**): ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.98 (t, *J* = 5.6 Hz, 2H), 3.18–3.13 (m, 4H), 1.51–1.44 (m, 4H), 1.29–1.25 (m, 4H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 161.4, 93.0, 38.9, 27.0, 25.3. The obtained NMR spectra are consistent with the reported data.[S2]

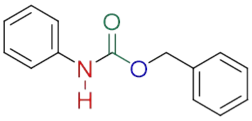


2,2,2-Trichloro-*N*-(4-{[4-(2,2,2-trichloroacetamido) phenyl]methyl}phenyl)acetamide (**3j**): ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.77 (s, 2H), 7.55 (d, *J* = 8.3 Hz, 4H), 7.24 (d, *J* = 8.3 Hz 4H), 3.91 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 159.7, 138.4, 135.2, 129.1, 129.0, 121.7, 93.1. The obtained NMR spectra are consistent with the reported data.[S2]

4. Preparation of compounds 5, 6

Experimental procedure for the synthesis of compound 5

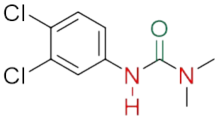
An aqueous chlorine dioxide solution was prepared by dissolving sodium chlorite ($NaClO_2$, 200 mg, 2.0 mmol (1.6 mmol of $ClO_2^{\bullet}$))[S1] and 35% hydrochloric acid (100 µL) in purified water (5 mL), and placed in chamber A. Chamber B was charged with 1-chloro-4-(trifluoromethyl)benzene (PCBTF, 1 mL) and tetrachloroethylene (51.5 µL, 0.5 mmol). After sealing, the entire H-shaped tube was irradiated with 405 nm LED light (90 mW cm^{-2}) for 2 h at room temperature. Subsequently, a solution of aniline (54.8 µL, 0.6 mmol) and pyridine (80.8 µL, 1.0 mmol) in MeCN (1 mL) was added to chamber B, and the mixture was stirred for 1 h. The reaction mixture in chamber B was quenched with saturated aqueous $NaHCO_3$, extracted with chloroform, and the organic layer was dried over anhydrous magnesium sulfate ($MgSO_4$). After evaporation of the solvent under reduced pressure, the resulting residue was transferred into a test tube, followed by the addition of MeCN (1 mL), benzyl alcohol (62 µL, 0.6 mmol), and DBU (89 µL, 0.6 mmol). The reaction mixture was then heated at 80 °C for 24 h with stirring. After cooling to room temperature, the mixture was extracted with $CHCl_3$, and the organic phase was dried over anhydrous $MgSO_4$. The solvent was evaporated under reduced pressure, and the crude product was purified by column chromatography to afford the desired product.



Benzyl *N*-phenylcarbamate (**5**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37–7.22 (m, 9H), 7.05 (t, *J* = 7.3 Hz, 1H), 6.77 (br, 1H), 5.18 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): 153.3, 137.7, 136.0, 129.0, 128.6, 128.3, 128.2, 123.4, 118.7, 66.9. The obtained NMR spectra are consistent with the reported data.[S2]

Experimental procedure for the synthesis of compound 6

An aqueous chlorine dioxide solution was prepared by dissolving sodium chlorite ($NaClO_2$, 200 mg, 2.0 mmol (1.6 mmol of $ClO_2^{\bullet}$))[S1] and 35% hydrochloric acid (100 µL) in purified water (5 mL), and placed in chamber A. Chamber B was charged with 1-chloro-4-(trifluoromethyl)benzene (PCBTF, 1 mL) and tetrachloroethylene (51.5 µL, 0.5 mmol). After sealing, the entire H-shaped tube was irradiated with 405 nm LED light (90 mW cm^{-2}) for 2 h at room temperature. Subsequently, a solution of 3,4-dichloroaniline (97 mg, 0.6 mmol) and pyridine (80.8 µL, 1.0 mmol) in MeCN (1 mL) was added to chamber B, and the mixture was stirred for 1 h. The reaction mixture in chamber B was quenched with saturated aqueous $NaHCO_3$, extracted with chloroform, and the organic layer was dried over anhydrous magnesium sulfate ($MgSO_4$). After evaporation of the solvent under reduced pressure, the resulting residue was transferred into a test tube, followed by the addition of MeCN (1 mL), 8% dimethylamine in MeCN (1.85 mL, 2.5 mmol), and DBU (373 µL, 2.5 mmol). The reaction mixture was then heated at 80 °C for 24 h with stirring. After cooling to room temperature, the mixture was extracted with $CHCl_3$, and the organic phase was dried over anhydrous $MgSO_4$. The solvent was evaporated under reduced pressure, and the crude product was purified by column chromatography to afford the desired product.

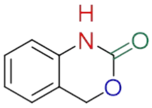


3-(3,4-Dichlorophenyl)-1,1-dimethylurea (**6**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (s, 1H), 7.30 (d, *J* = 8.8 Hz, 1H), 7.22 (d, *J* = 8.8 Hz, 1H), 6.44 (s, 1H), 3.02 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): 155.1, 138.8, 132.4, 130.2, 125.9, 121.3, 119.0, 36.4. The obtained NMR spectra are consistent with the reported data.[S5]

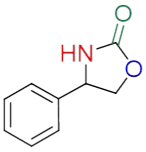
5. Preparation of compounds 7, 8

Experimental procedure

An aqueous chlorine dioxide solution was prepared by dissolving sodium chlorite ($NaClO_2$, 200 mg, 2.0 mmol (1.6 mmol of $ClO_2^{\bullet}$))[S1] and 35% hydrochloric acid (100 μL) in purified water (5 mL), and placed in chamber A. Chamber B was charged with 1-chloro-4-(trifluoromethyl)benzene (PCBTF, 1 mL) and tetrachloroethylene (51.5 μL, 0.5 mmol). After sealing, the entire H-shaped tube was irradiated with 405 nm LED light (90 mW cm^{-2}) for 2 h at room temperature. Subsequently, a solution of amino alcohol (0.6 mmol) and pyridine (80.8 μL, 1.0 mmol) in MeCN (1 mL) was added to chamber B, and the mixture was stirred for 1 h. The reaction mixture in chamber B was quenched with saturated aqueous $NaHCO_3$, extracted with chloroform, and the organic layer was dried over anhydrous magnesium sulfate ($MgSO_4$). After evaporation of the solvent under reduced pressure, the residue was purified by column chromatography to afford the desired product.



1,4-Dihydro-3,1-benzoxazin-2-one (**7**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (br, 1H), 7.27 (t, *J* = 7.8 Hz, 1H), 7.12 (d, *J* = 7.3 Hz, 1H), 7.06 (t, *J* = 7.3 Hz, 1H), 6.81 (d, *J* = 7.8 Hz, 1H), 5.32 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.6, 135.5, 129.2, 124.2, 123.3, 117.9, 114.2, 68.7. The obtained NMR spectra are consistent with the reported data.[S6]

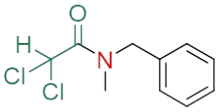


4-Phenyl-2-oxazolidinone (**8**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42–7.32 (m, 5H), 6.43 (br, 1H), 4.95 (d, *J* = 7.3 Hz, 1H), 4.79 (d, *J* = 8.7, 1H), 4.16 (dd, *J* = 8.7, 7.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.0, 139.5, 129.1, 128.7, 126.0, 74.5, 56.3. The obtained NMR spectra are consistent with the reported data.[S7]

6. Preparation of compound 10

Experimental procedure

An aqueous chlorine dioxide solution was prepared by dissolving sodium chlorite ($NaClO_2$, 200 mg, 2.0 mmol (1.6 mmol of $ClO_2^{\bullet}$))[S1] and 35% hydrochloric acid (100 µL) in purified water (5 mL), and placed in chamber A. Chamber B was charged with 1-chloro-4-(trifluoromethyl)benzene (PCBTF, 1 mL) and trichloroethylene (48.4 µL, 0.5 mmol). After sealing, the entire H-shaped tube was irradiated with 405 nm LED light (90 mW cm^{-2}) for 2 h at room temperature. Subsequently, a solution of *N*-methylbenzylamine (73 mg, 0.6 mmol) and pyridine (80.8 µL, 1.0 mmol) in MeCN (1 mL) was added to chamber B, and the mixture was stirred for 1 h. The reaction mixture in chamber B was quenched with saturated aqueous $NaHCO_3$, extracted with chloroform, and the organic layer was dried over anhydrous magnesium sulfate ($MgSO_4$). After evaporation of the solvent under reduced pressure, the residue was purified by column chromatography to afford the desired product.



N-Benzyl-2,2-dichloro-*N*-methylacetamide (**10**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35–7.23 (m, 5H), 6.29 (s, 0.68H), 6.26 (s, 0.32H), 4.72 (s, 0.75H), 4.61 (s, 1.25H), 3.11 (s, 1.95H), 2.96 (s, 1.05H); ^{13}C NMR (100 MHz, $CDCl_3$): Major δ; 163.7, 135.8, 128.8, 127.9, 65.5, 52.3, 35.1., Minor δ; 163.7, 135.1, 129.1, 128.1, 127.8, 126.6, 65.1, 53.5, 35.0. HRMS (ESI) m/z: $[M + Na]^+$ calcd. for $C_{10}H_{11}Cl_2NNaO$: 254.0110, found: 254.0113. The obtained NMR spectra are consistent with the reported data.[S8]

7. Gram-scale experiment

Experimental procedure

An aqueous chlorine dioxide solution was prepared by dissolving sodium chlorite ($NaClO_2$, 1625 mg, 16.3 mmol (13.0 mmol of $ClO_2^{\bullet}$))[1] and 35% hydrochloric acid (1.3 mL) in purified water (60 mL), and placed in chamber A. Chamber B was charged with 1-chloro-4-(trifluoromethyl)benzene (PCBTF, 13 mL) and tetrachloroethylene (1085 mg, 6.5 mmol). After sealing, the entire H-shaped tube was irradiated with 405 nm LED light (90 mW cm^{-2}) for 2 h at room temperature. Subsequently, a solution of *N*-methylbenzylamine (1011 µL, 7.8 mmol) and pyridine (1050 µL, 13.0 mmol) in MeCN (13 mL) was added to chamber B, and the mixture was stirred for 1 h. The reaction mixture in chamber B was quenched with saturated aqueous $NaHCO_3$, extracted with chloroform, and the organic layer was dried over anhydrous magnesium sulfate ($MgSO_4$). After evaporation of the solvent under reduced pressure, the residue was purified by column chromatography to afford the desired amide product (1291.1 mg, 75 %).

8. References

S1) The concentration of $ClO_2^{\bullet}$ was estimated by UV–vis spectroscopy in aqueous solution using a reported molar absorption coefficient (ε_{360nm} = 1,150 M^{-1} cm^{-1}), see : E. M. Aieta, J. D. Berg, *J. Am. Water Works Assoc.*, 1986, **78**, 62–72.

S2) T. Akamatsu, M. Shele, A. Matsune, Y. Kashiki, F. Liang, T. Okazoe, A Tsuda, *ACS Omega*, 2023, **8**, 2669–2684.

S3) T. Naito, A. Saito, M. Ueda, O. Miyata, *Heterocycles*, 2005, **65**, 1857–1869.

S4) Q. Zhao, B. Li, X. Zhou, Z. Wang, F.-L. Zhang, Y. Li, X. Zhou, Y. Fu, Y.-F. Wang, *J. Am. Chem. Soc.*, 2022, **144**, 15275−15285.

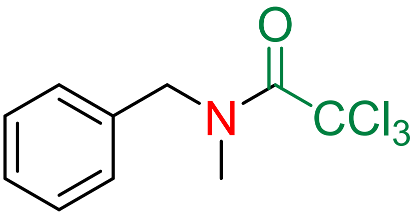
S5) I. Degani, R. Fochi, C. Magistris, M. Migliaccio, *Synthesis*, 2009, **5**, 801-808.

S6) L. Rena, N. Jiao, *Chem. Commun*., 2014, **50**, 3706–3709.

S7) Y. Liu, Z. Yi, X. Yang, H. Wang, C. Yin, M. Wang, X.-Q. Dong, X. Zhang, *ACS Catal.*, 2020, **10**, 11153–11161.

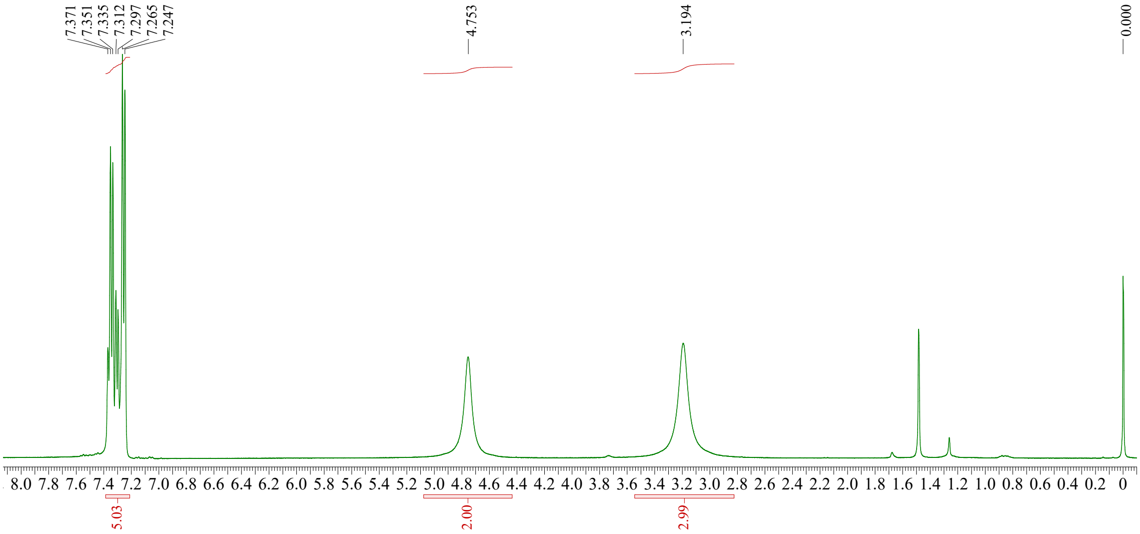
S8) Y. Liu, S. G. Bender, D. Sorigue, D. J. Diaz, A. D. Ellington, G. Mann, S. Allmendinger, and T. K. Hyster, *J. Am. Chem. Soc.*, 2024, **146**, 7191−7197.

9. NMR graphics of new compounds

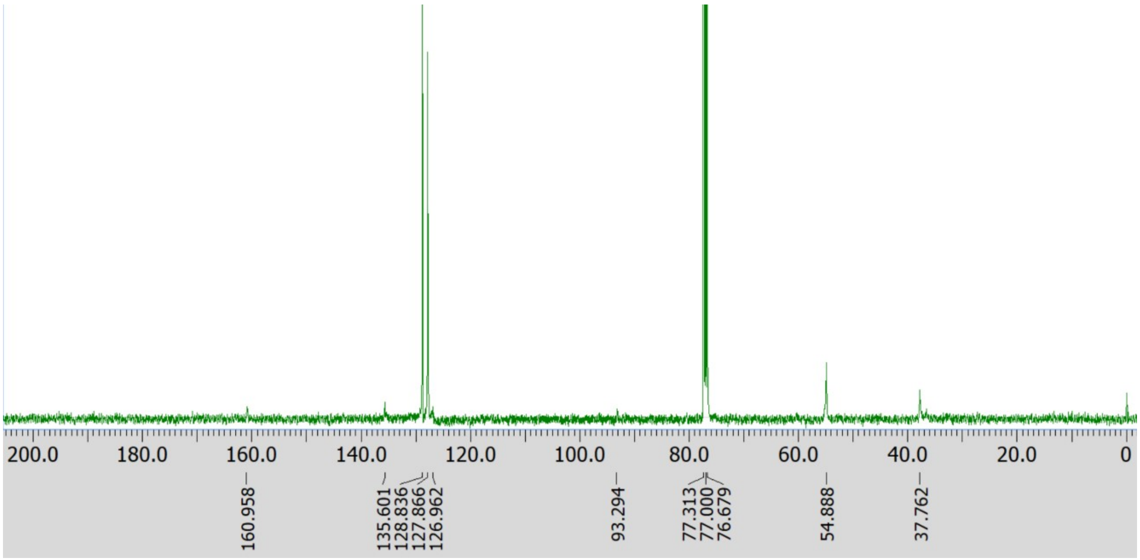


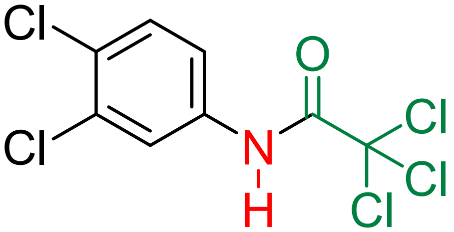
3a

Proton



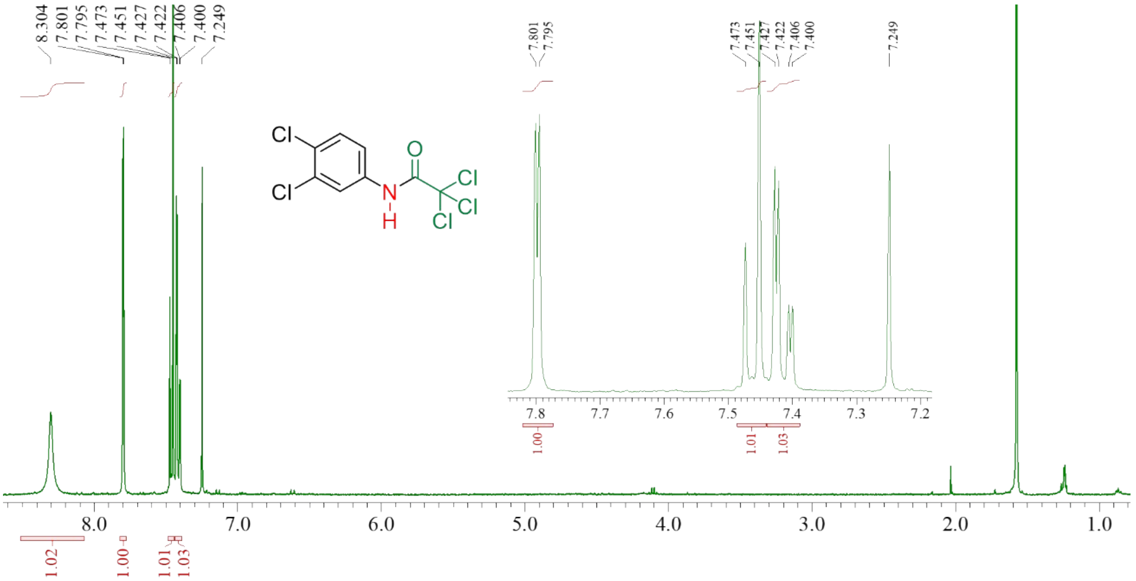
Carbon



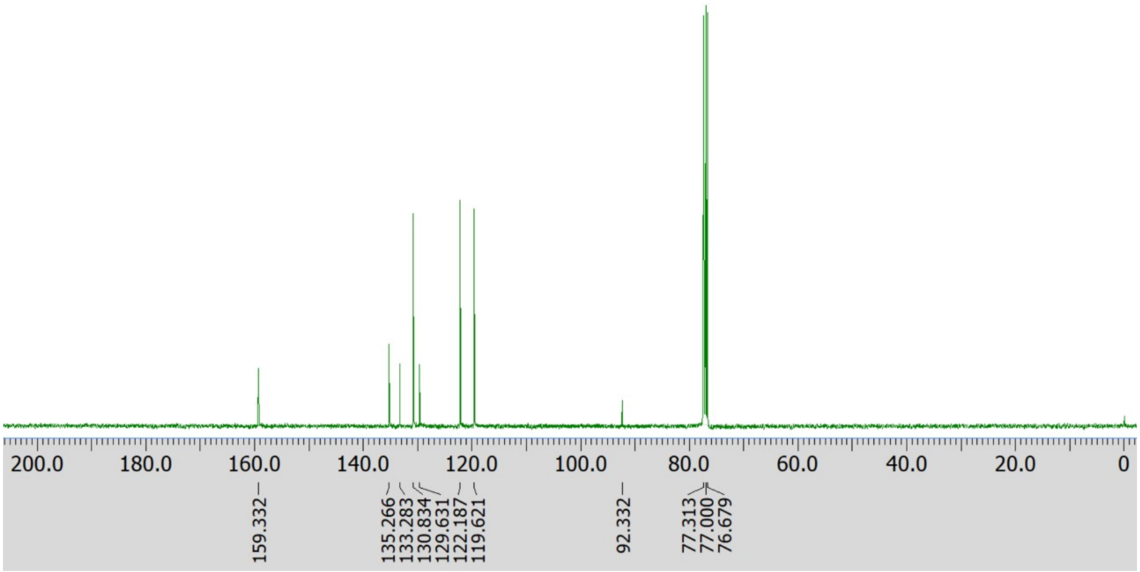


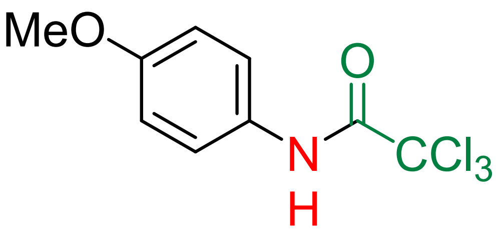
3g

Proton



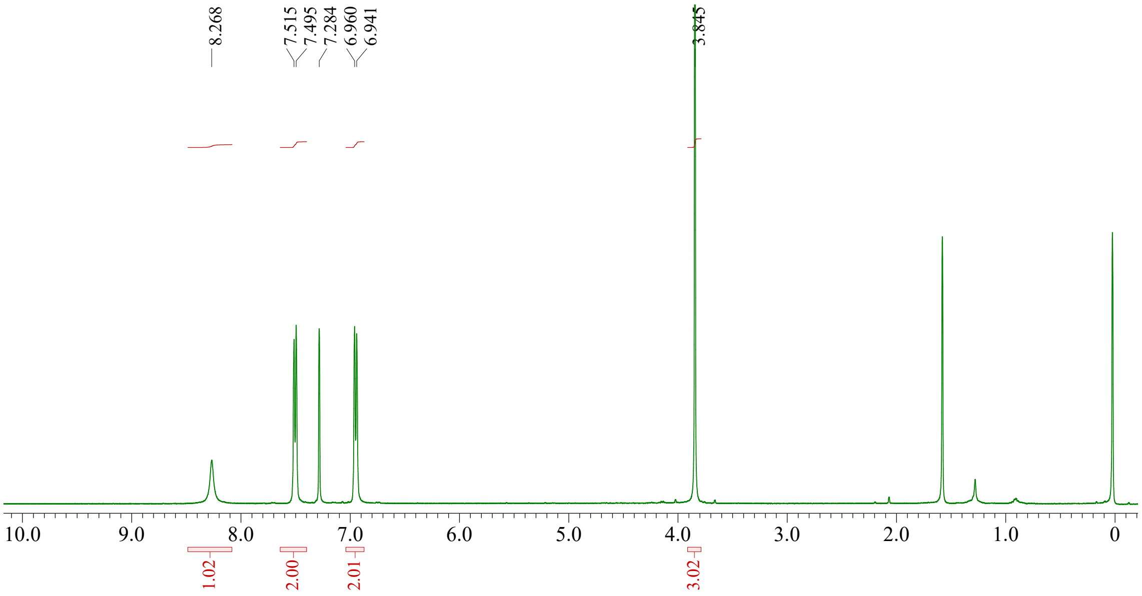
Carbon



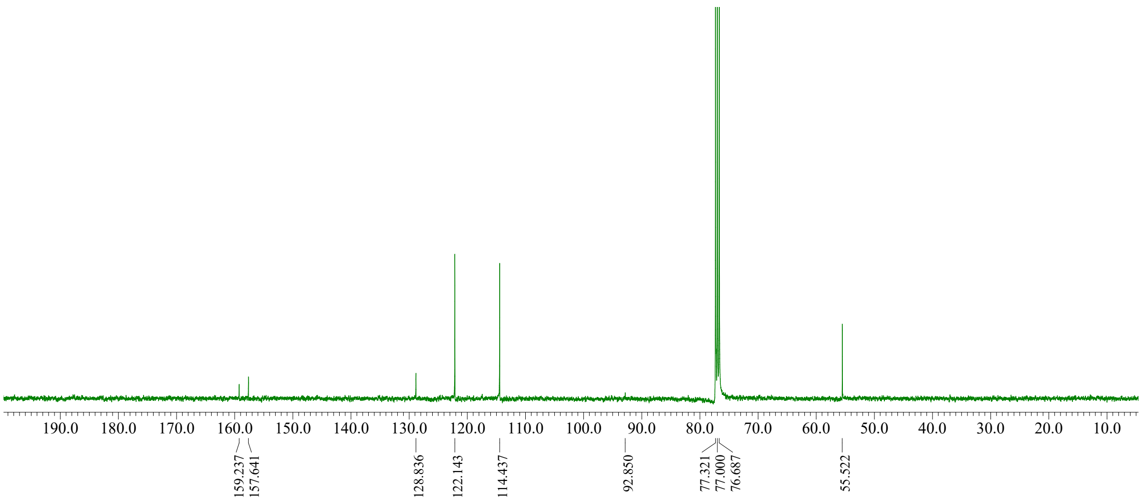


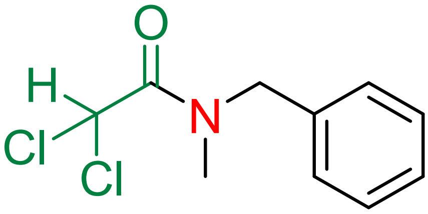
3h

Proton



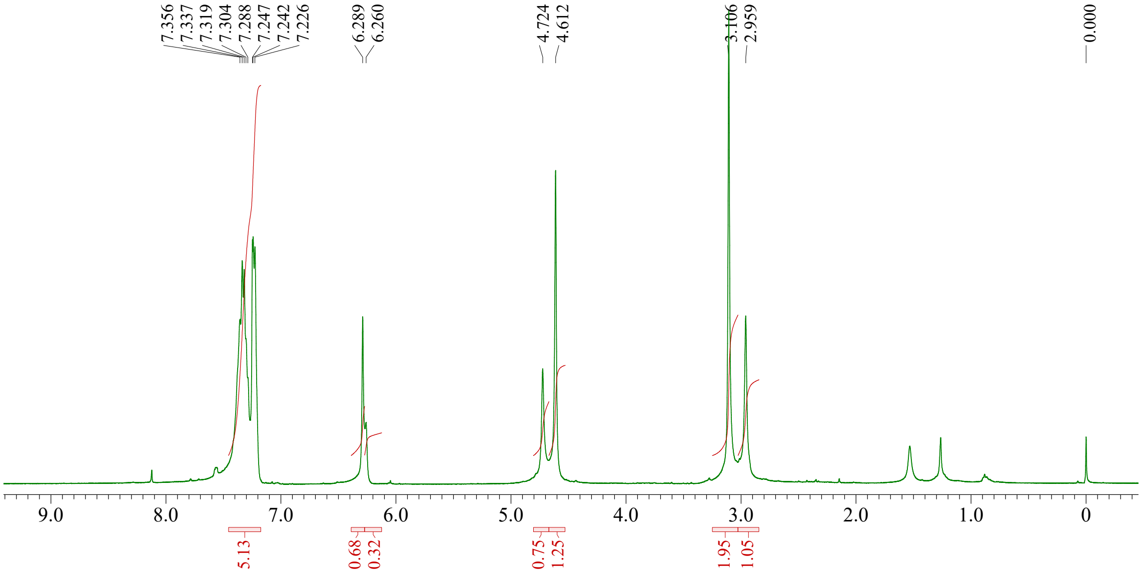
Carbon



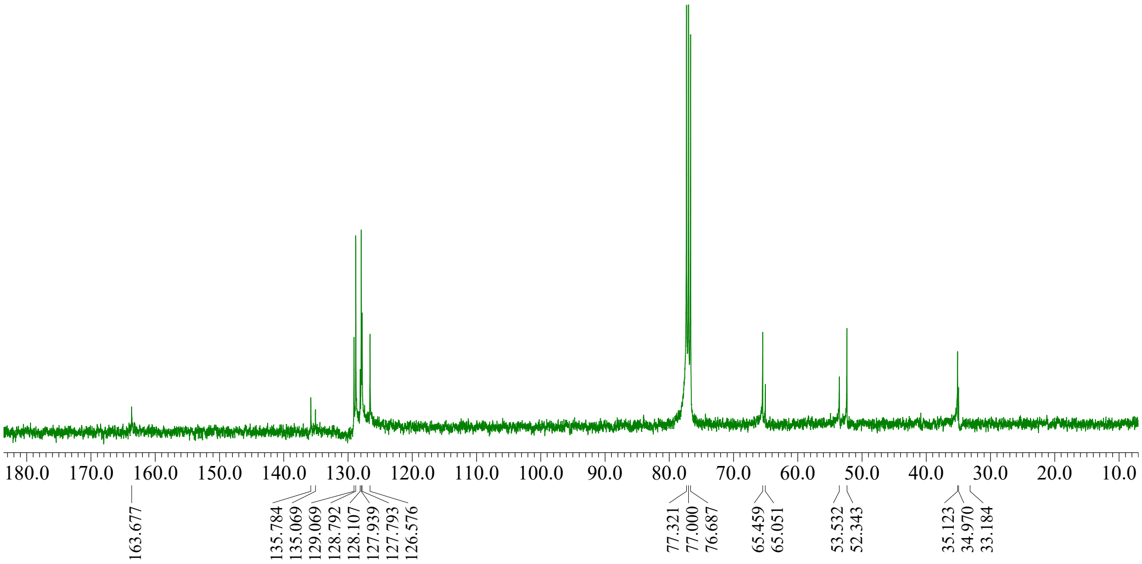


10

Proton



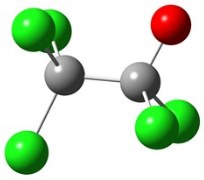
Carbon



10. DFT calculation information

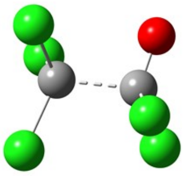
All DFT calculations were carried out with Gaussian 16 (Revision C.02, Gaussian, Inc., Wallingford, CT, USA)[1]. Geometry optimizations for all ground-state species and transition states were performed using the B3LYP functional in combination with the 6-311+G(2d) basis set. Vibrational frequency analyses were conducted at the same level of theory to characterize each stationary point: minima were confirmed to have no imaginary frequencies, whereas transition states were verified to possess only one imaginary frequency corresponding to motion along the reaction coordinate. Thermal corrections obtained from the frequency calculations were added to the electronic energies to afford Gibbs free energies (*G*) at 298.15 K. For each transition state, intrinsic reaction coordinate (IRC) calculations were performed to confirm that the optimized transition structure connects the corresponding reactant and product on the potential energy surface.

1. Gaussian 16, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, Gaussian, Inc. Wallingford CT, **2019**.



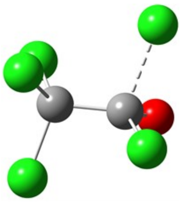
Electronic Energy = –2452.5077 Hartree

Atom	x	y	z
C	-0.70294770	0.01382188	0.05325604
C	0.79778648	-0.03609160	-0.44421273
Cl	-1.45155187	1.55118281	-0.46351690
Cl	-1.56343345	-1.34180619	-0.74641456
Cl	-0.81479821	-0.14240901	1.82423446
Cl	1.74601516	1.40880898	0.22082223
Cl	1.59795246	-1.56652498	0.10905597
O	0.96122973	0.20954261	-1.71316756



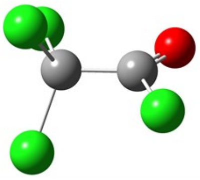
Electronic Energy = –2452.5026 Hartree (Imaginary Frequency = –436.18)

Atom	x	y	z
C	0.77052717	-0.00000821	0.07272935
Cl	1.57307170	-1.45799985	-0.51879409
Cl	1.57307193	1.45811736	-0.51846371
Cl	0.66748129	-0.00020723	1.82935269
Cl	-1.71700355	-1.47856673	0.11629564
Cl	-1.71700364	1.47854060	0.11663055
O	-0.72341541	0.00020407	-1.80811214
C	-0.88155682	0.00006432	-0.56613958



Electronic Energy = –2452.5060 Hartree (Imaginary Frequency = –327.59)

Atom	x	y	z
C	0.71650838	-0.07789144	0.05191058
C	-0.72479561	0.21061001	-0.52234138
Cl	1.27315906	-1.68107713	-0.48706695
Cl	1.78015682	1.18063228	-0.66995610
Cl	0.77081288	0.02374614	1.82703863
Cl	-1.96014137	-1.27168942	0.21419012
Cl	-1.39570381	1.76053709	0.08028053
O	-0.98888718	-0.12535545	-1.69671015

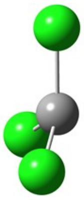


Electronic Energy = –1992.3617 Hartree

Atom	x	y	z
C	0.46592385	-0.05941364	-0.00000000
C	-0.79320048	0.86084768	0.00000014
Cl	1.93071840	0.94807125	0.00000042
Cl	0.43510447	-1.07785592	1.47265266
Cl	0.43510467	-1.07785502	-1.47265329
Cl	-2.33159353	-0.03392371	0.00000006
O	-0.75187731	2.03724671	0.00000022

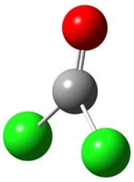
Electronic Energy = –460.1671 Hartree

Atom	x	y	z
Cl	0.00000000	0.00000000	0.00000000



Electronic Energy = –1418.7295 Hartree

Atom	x	y	z
C	-0.00000136	0.00000029	0.27594507
Cl	-1.66864775	0.31181173	-0.03246419
Cl	1.10436142	1.28918346	-0.03246410
Cl	0.56428681	-1.60099529	-0.03246409



Electronic Energy = –1033.8182 Hartree

Atom	x	y	z
Cl	0.00000000	1.46023958	0.48357661
Cl	0.00000000	-1.46023958	0.48357661
O	-0.00000000	0.00000000	-1.67694125
C	0.00000000	0.00000000	-0.50434580