Visible Light Driven Copper(II) Catalyzed Aerobic Oxidative Cleavage of Carbon−Carbon Bond: A Combined Experimental and Theoretical Study

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Supporting Information

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1. General information

Column chromatography was carried out with *silica gel* 60 (particle size 0.040–0.063 mm, 230–400 mesh) and commercially available solvents. Thin-layer chromatography (TLC) was conducted on aluminum sheets coated with *silica gel* 60 F254 with visualization by a UV lamp (254 or 360 nm).

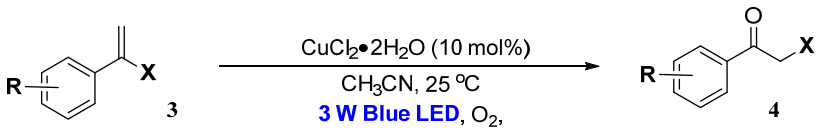
^{1}H and ^{13}C NMR spectra were recorded at 300 and 75 MHz at 25 °C with a 300 MHz instrument. Chemical shifts are reported in parts per million (ppm), using the residual solvent signal as an internal standard: $CDCl_3$ (^{1}H NMR: δ 7.26, singlet; ^{13}C NMR: δ 77.0, triplet). Multiplicities were given as: *s* (singlet), *d* (doublet), *t* (triplet), *q* (quartet), *quintet*, *m* (multiplets), *dd* (doublet of doublets), *dt* (doublet of triplets), and *br* (broad). Coupling constants (*J*) were recorded in Hertz (Hz). The number of proton atoms (*n*) for a given resonance was indicated by *n*H. The number of carbon atoms (*n*) for a given resonance was indicated by *n*C. HRMS was reported in units of mass of charge ratio (m/z). Mass samples were dissolved in DCM and MeOH (HPLC Grade) unless otherwise stated. Electrochemical measurements were carried out by cyclic voltammetry (CV). The cyclic voltammetry was performed with an Autolab potentiostat by Echochemie under nitrogen atmosphere in a one-compartment electrolysis cell consisting of a platinum wire working electrode, a platinum wire counter electrode, and a quasi Ag/AgCl reference electrode. Cyclic voltammograms were monitored at scan rates of either 100 $mV \bullet s^{-1}$ or 50 $mV \bullet s^{-1}$ and recorded in distilled acetonitrile. The concentration of the complex was maintained at 0.5 mM or less and each solution contained 0.1 M of tetrabutylammonium hexafluorophosphate (TBAP) as the electrolyte.

2. General experimental procedure for the $CuCl_2·2H_2O$–Catalyzed Aerobic Photooxygenation of Diverse Styrenes

1 **2**

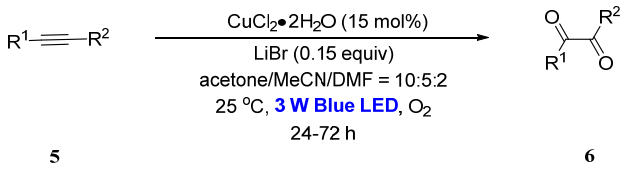
3.4 mg (0.02 mmol, 0.1 equiv) of $CuCl_2·2H_2O$, **1** (0.2 mmol, 1.0 equiv), and 0.85 mg of LiCl (0.02 mmol, 0.1 equiv) was added into a 10.0 mL sample vial, and the reaction mixture was removed in vacuo, then 2.0 mL CH_3CN was sequentially added. The reaction mixture was stirred at 25 °C under an oxygen atmosphere (The sample vial was fitted with an oxygen balloon and the temperature was maintained in an incubator) and irradiated by a 3 W blue LED (λ = 450–455 nm). The reaction was monitored by TLC. Upon complete consumption of **1**, the solvent was removed *in vacuo.* The reaction mixture was then loaded onto a short *silica gel* column, followed by gradient elution with petroleum ether/ethyl acetate (50/1–10/1 ratio), then concentrated the solvent *in vacuo* to afford products.

3. General experimental procedure for the $CuCl_2 \cdot 2H_2O$–Catalyzed Aerobic Photooxygenation of Vinyl Halides



3.4 mg (0.02 mmol, 0.1 equiv) of $CuCl_2 \cdot 2H_2O$, and **3** (0.2 mmol, 1.0 equiv), was added into a 10.0 mL sample vial, and the reaction mixture was removed *in vacuo*, then 2.0 mL CH_3CN (HPLC Grade) was added. The reaction mixture was stirred at 25 °C under an oxygen atmosphere (The sample vial was fitted with an oxygen balloon and the temperature was maintained in an incubator) and irradiated by a 3 W blue LED (λ = 450–455 nm). The reaction was monitored by TLC. Upon complete consumption of **3**, the solvent was removed *in vacuo*. The reaction mixture was then loaded onto a short *silica gel* column, followed by gradient elution with petroleum ether/ethyl acetate (50/1–10/1 ratio), then concentrated the solvent *in vacuo* to afford products.

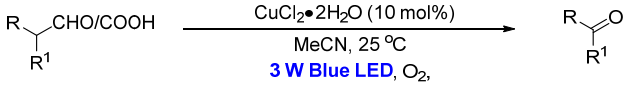
4. General experimental procedure for the $CuCl_2·2H_2O$–Catalyzed Aerobic Photooxygenation of Alkynes



5 **6**

5.2 mg (0.03 mmol, 0.15 equiv) of $CuCl_2·2H_2O$, **5** (0.2 mmol, 1.0 equiv), and 2.6 mg of LiBr (0.03 mmol, 0.15 equiv) was added into a 10.0 mL sample vial, and the reaction mixture was removed in vacuo, then 1.7 mL of solvent (actone:CH_3CN:DMF = 10:5:2) was added. The reaction mixture was stirred at 25 °C under an oxygen atmosphere (The sample vial was fitted with an oxygen balloon and the temperature was maintained in an incubator) and irradiated by a 3 W blue LED (λ = 450–455 nm). The reaction was monitored by TLC. Upon complete consumption of **5**, the solvent was removed *in vacuo.* The reaction mixture was then loaded onto a short *silica gel* column, followed by gradient elution with petroleum ether/ethyl acetate (100/1–10/1 ratio), then concentrated the solvent *in vacuo* to afford products.

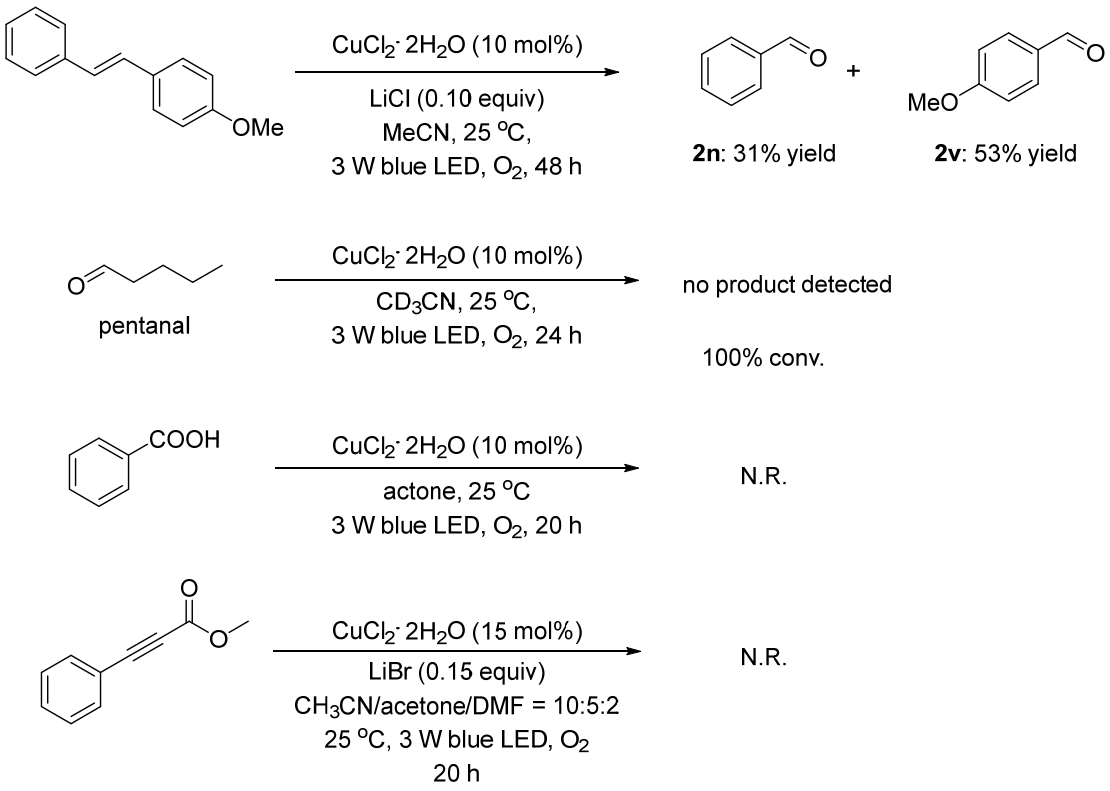
5. General experimental procedure for the $CuCl_2·2H_2O$–Catalyzed Aerobic Photooxygenation of Aldehydes and Carboxylic Acids



7/8 **2**

3.4 mg (0.02 mmol, 0.1 equiv) of $CuCl_2·2H_2O$, and aldehydes or carboxylic acids (0.2 mmol, 1.0 equiv), was added into a 10.0 mL sample vial, and the reaction mixture was removed in *vacuo*, then 2.0 mL MeCN was sequentially added. The reaction mixture was stirred at 25 °C under an oxygen atmosphere (The sample vial was fitted with an oxygen balloon and the temperature was maintained in an incubator) and irradiated by a 3 W blue LED (λ = 450–455 nm). The reaction was monitored by TLC. Upon complete consumption of **7/8**, the solvent was removed *in vacuo*, the reaction mixture was then loaded onto a short *silica gel* column, followed by gradient elution with petroleum ether/ethyl acetate (50/1–10/1 ratio), then concentrated the solvent *in vacuo* to afford products.

6. Other examined substrates

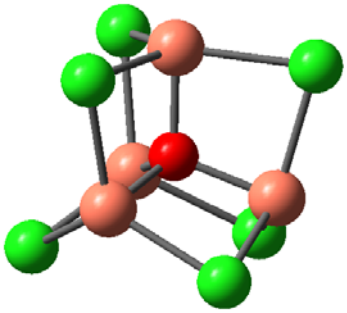
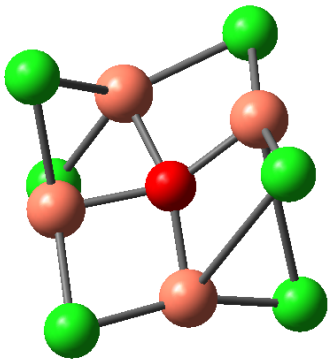
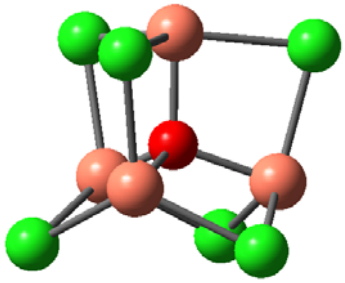
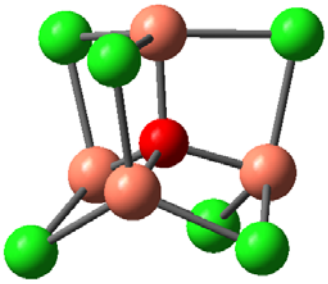


7. Computational Details

Density functional theory (DFT) modelling was carried out with Gaussian 16 computational chemistry suite.[1] Geometries of gas-phase minimum and transition state (TS) electronic structures were optimized with the M06 functional,[2] with Pople's basis-set 6-31G(d,p).[3] Frequency calculations were carried out at that level to ensure convergence (all positive eigenvalues for minima and single negative for TS structures). Thermal corrections were determined at the gas-phase M06/6-31G(d,p) level using the unscaled frequencies - $G_{correction}$ and $H_{correction}$ for free energy and enthalpy respectively. Gas-phase single point calculations at M06 and Dunning's aug-cc-pVTZ basis-set,[4–8] were carried out to determine the more accurate electronic energy ($E_{M06/aug\text{-}cc\text{-}pVTZ}$). Solvation free energies (ΔG_{solv}) were considered with the PCM model (acetonitrile parameters),[9] on the optimized structures at M06/aug-cc-pVDZ level of theory. The reported solution free energy, G_{sol}, is the sum of $E_{M06/aug\text{-}cc\text{-}pVTZ}$, ΔG_{solv} and gas-phase thermal correction.

The structures of $[Cu_4OCl_6]$ cluster of different spin states were considered. The low spin singlet (open-shell or OS) structure was calculated with the broken symmetry approach or antiferromagnetic coupling procedure for which the wavefunction was first stabilized (stable=opt). Then with the stable wavefunction as guess, the structure was optimized accordingly. The singlet (closed-shell or CS) was calculated with normal DFT procedures which yielded an unsymmetrical structure with large deviations in Cu-Cl bond distances. The energy of structure optimized by singlet (CS) method is most unstable amongst all. The structure of cluster optimized with the singlet (OS) approach is more symmetrical and very similar to the structures of triplet and quintet high spin states (see table below). However, the quintet spin state was calculated to be most stable, and as such all DFT modelling was performed in using this multiplicity.

Multiplicity	3D structure	Energy (hartrees)	Average Cu-Cl bond (Å) + Std. Dev.	Average Cu-O bond (Å) + Std. Dev.

Singlet (OS)		-9397.313152	2.34 ± 0.01	1.84 ± 0.00
Singlet (CS)		-9397.241205	2.41 ± 0.42	1.86 ± 0.02
Triplet		-9397.250048	2.34 ± 0.00	1.85 ± 0.00
Quintet		-9397.316961	2.34 ± 0.00	1.84 ± 0.00

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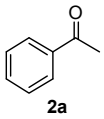
8. Table of Energies: Minimum and Transition State Structures

Species	$G_{correction}$	$H_{correction}$	$E_{M06/aug-cc-pVTZ}$	G_{gas}	ΔG_{solv}	G_{sol}
Chlorostyrene	hartrees	hartrees	hartrees	kcal/mol	kcal/mol	kcal/mol
***α*-chlorostyrene (c-sty)**	0.090766	0.132413	-769.1029472	-482555.14	-2.26	-482557.40
O2t	-0.01604	0.007235	-150.3026044	-94324.95	-0.05	-94325.00
pdt1	0.094293	0.139037	-844.3417883	-529765.30	-4.59	-529769.89
cpx1	-0.03763	0.032911	-9398.801785	-5897771.73	-16.30	-5897788.03
cpx1 + sty	0.053134	0.165324	-10167.90473	-6380326.88	-18.56	-6380345.44
cpx1 + O2 + c-sty	0.037097	0.172559	-10318.20734	-6474651.83	-18.61	-6474670.44
cpx2	0.07185	0.167256	-10167.94178	-6380338.38	-17.13	-6380355.51
TS1	0.074249	0.165431	-10167.93202	-6380330.75	-18.4	-6380349.15
cpx3	0.073544	0.166625	-10167.93924	-6380335.73	-16.86	-6380352.59
cpx4	0.075335	0.176216	-10318.23295	-6474643.90	-24.79	-6474668.69
TS2	0.077908	0.174545	-10318.22189	-6474635.35	-22.88	-6474658.23
cpx5	0.084626	0.17778	-10318.27203	-6474662.59	-18.4	-6474680.99
TS3	0.084859	0.176859	-10318.26385	-6474657.31	-14.2	-6474671.51
cpx6	0.084184	0.178081	-10318.27803	-6474666.64	-17.83	-6474684.47
cpx7	0.080646	0.178465	-10318.27727	-6474668.38	-14.84	-6474683.22
TS4	0.078688	0.176463	-10318.24835	-6474651.46	-16.34	-6474667.80
cpx8	0.080092	0.179036	-10318.2919	-6474677.91	-19.22	-6474697.13
TS5	0.078729	0.176745	-10318.26194	-6474659.97	-15.00	-6474674.97
TS3a	0.076949	0.175726	-10318.18552	-6474613.13	-16.12	-6474629.25
cpx9	0.084242	0.177975	-10318.30919	-6474686.16	-13.08	-6474699.24
int5 - pdt1 + c-sty	0.080715	0.171351	-10243.07035	-6427475.997	-10.75	-6427486.75

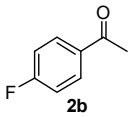
cpx10	0.076168	0.171189	-10243.05462	-6427468.98	-13.66	-6427482.64
TS6	0.077692	0.169939	-10243.04098	-6427459.46	-20.65	-6427480.11
cpx11	0.080229	0.171624	-10243.0899	-6427488.57	-17.17	-6427505.74
TS7	0.077038	0.170009	-10243.078	-6427483.10	-17.59	-6427500.69
cpx1 + pdt1	0.056661	0.171948	-10243.14357	-6427537.04	-20.89	-6427557.93
cpx1a	0.073481	0.167771	-10167.94562	-6380339.77	-15.10	-6380354.87
cpx1a + O2	0.057444	0.175006	-10318.24822	-6474664.71	-15.15	-6474679.86
TS1a	0.078328	0.174447	-10318.20878	-6474626.86	-17.39	-6474644.25
cpx2a	0.08127	0.177059	-10318.23091	-6474638.90	-13.18	-6474652.08
TS2a	0.082998	0.175457	-10318.21933	-6474630.55	-14.20	-6474644.75
cpx3a	0.082541	0.176831	-10318.21957	-6474630.99	-17.69	-6474648.68
cpx6a	0.082389	0.177954	-10318.26159	-6474657.45	-17.13	-6474674.58
TS4a	0.081157	0.175427	-10318.19444	-6474616.08	-27.21	-6474643.29
Methylstyrene	hartrees	hartrees	hartrees	kcal/mol	kcal/mol	kcal/mol
***α*-methylstyrene (m-sty)**	0.128215	0.169955	-348.7965871	-218789.40	-2.04	-218791.44
ketone (ket)	0.105091	0.146432	-384.7455686	-241361.90	-4.54	-241366.44
aldehyde (ald)	0.005609	0.030423	-114.4797952	-71832.55	-3.37	-71835.92
cpx1 + m-sty	0.090583	0.202866	-9747.598373	-6116561.14	-18.34	-6116579.48
cpx1 + O2 + m-sty	0.074546	0.210101	-9897.900977	-6210886.09	-18.39	-6210904.48
cpx2b	0.109609	0.204828	-9747.639128	-6116574.77	-17.07	-6116591.84
TS1b	0.111011	0.20277	-9747.633892	-6116570.61	-16.99	-6116587.60
cpx3b	0.110922	0.204202	-9747.63687	-6116572.53	-17.55	-6116590.08
cpx4b	0.116014	0.214555	-9897.93415	-6210880.88	-26.1	-6210906.98
TS2b	0.115599	0.211959	-9897.924916	-6210875.35	-16.99	-6210892.34

cpx5b	0.121448	0.215405	-9897.970204	-6210900.09	-19.76	-6210919.85
TS3b	0.122314	0.214414	-9897.958051	-6210891.92	-18.12	-6210910.04
cpx6b	0.122104	0.215777	-9897.972602	-6210901.19	-19.4	-6210920.59
cpx7b	0.121801	0.215852	-9897.96334	-6210895.57	-17.19	-6210912.76
TS4b	0.118652	0.213152	-9897.901478	-6210858.72	-25.77	-6210884.49
cpx8b	0.121449	0.215328	-9897.943044	-6210883.05	-16.6	-6210899.65
LiCl	-0.01935	0.004848	-467.8023953	-293558.15	-41.54	-293599.69
cpx7b_LiCl	0.11738	0.222107	-10365.80194	-6504467.06	-49.65	-6504516.71
TS4b_LiCl	0.117008	0.220307	-10365.77705	-6504451.68	-39.25	-6504490.93
Cl-	-0.01502	0.00236	-460.2683751	-288827.83	-68.57	-288896.40
cpx7b_Cl	0.115943	0.218813	-10358.35112	-6499792.57	-41.93	-6499834.50
TS4b_Cl	0.118529	0.216605	-10358.30064	-6499759.27	-47.43	-6499806.70
TS5b	0.117316	0.213946	-9897.955942	-6210893.74	-19.76	-6210913.50
cpx8b	0.122402	0.215276	-9897.981815	-6210906.78	-16.52	-6210923.30
TS5b	0.115719	0.212745	-9898.041089	-6210948.17	-15.24	-6210963.41
cpx9b	0.119833	0.216458	-9897.971218	-6210901.74	-16.9	-6210918.64
TS5b	0.117289	0.213197	-9897.918307	-6210870.14	-16.88	-6210887.02
int1 + ket + ald	0.073068	0.209766	-9898.027149	-6210966.19	-24.21	-6210990.40
cpx3c	0.113419	0.21305	-9897.912137	-6210868.70	-14.51	-6210883.21
TS1c	0.115345	0.211766	-9897.901466	-6210860.79	-17.81	-6210878.60
cpx4c	0.118947	0.215324	-9897.96877	-6210900.76	-19.18	-6210919.94

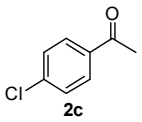
9. Characterization data of products



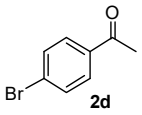
Colorless oil; 73% yield (from 1a, 17.6 mg); 83% yield (from **7a**, 20 mg); 87 yield (from **8a**, 21 mg) ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04–7.88 (m, 2H), 7.54 (ddd, *J* = 6.5, 3.8, 1.2 Hz, 1H), 7.43 (dd, *J* = 10.3, 4.6 Hz, 2H), 2.58 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.1, 136.9, 133.0, 128.5, 128.2, 26.5.



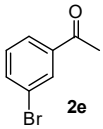
Colorless oil; 70% yield (from **1b**, 19.3 mg); 80% yield (from **8b**, 22 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07–7.86 (m, 2H), 7.18–7.01 (m, 2H), 2.57 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.5, 165.7 (d, *J* = 254.6 Hz), 133.4 (d, *J* = 3.0 Hz), 130.9 (d, *J* = 9.4 Hz), 115.6 (d, *J* = 21.9 Hz), 26.5.



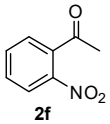
Colorless oil; 56% yield (16.7 mg); ^{1}H NMR (300 MHz, CDCl3) δ 7.94–7.79 (m, 2H), 7.48–7.32 (m, 2H), 2.57 (d, J = 1.3 Hz, 3H); ^{13}C NMR (75 MHz, CDCl3) δ 196.8, 139.4, 135.3, 129.6, 128.8, 26.5.



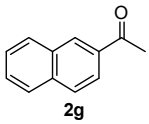
White soild; 72% yiled (28.7 mg); ^{1}H NMR (300 MHz, CDCl3) δ 7.87–7.71 (m, 2H), 7.63–7.49 (m, 2H), 2.55 (s, 3H); ^{13}C NMR (75 MHz, CDCl3) δ 196.9, 135.7, 131.8, 129.7, 128.2, 26.4.



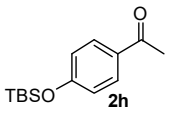
Colorless oil; 75% yield (29.7 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (t, *J* = 1.7 Hz, 1H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.72–7.64 (m, 1H), 7.34 (t, *J* = 7.9 Hz, 1H), 2.58 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.6, 138.7, 135.9, 131.3, 130.2, 126.8, 122.9, 26.6.



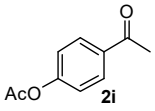
Yellow oil; 90% yield (29.2 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 8.2, 0.6 Hz, 0H), 7.71 (td, *J* = 7.5, 1.0 Hz, 0H), 7.59 (td, *J* = 8.1, 1.4 Hz, 0H), 7.42 (dd, *J* = 7.5, 1.2 Hz, 0H), 2.53 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.9, 145.6, 137.8, 134.2, 130.6, 127.2, 124.3, 30.1.



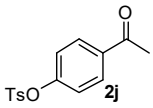
White soild; 84% yield (28.6 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.07–7.82 (m, 4H), 7.66–7.50 (m, 2H), 2.73 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.1, 135.5, 134.4, 132.4, 130.2, 129.5, 128.4, 128.4, 127.7, 126.7, 123.8, 26.7.



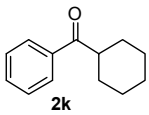
White solid; 62% yield (30.1 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.93–7.81 (m, 2H), 6.87 (t, *J* = 5.7 Hz, 2H), 2.55 (s, 3H), 0.98 (s, 9H), 0.22 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.9, 160.2, 130.8, 130.5, 119.8, 26.4, 25.5, 18.2, -4.4.



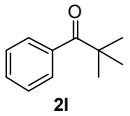
White solid; 88%yield (31.5 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.6 Hz, 2H), 7.18 (d, *J* = 8.6 Hz, 2H), 2.58 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.8, 168.9, 154.2, 134.6, 129.9, 121.7, 26.6, 21.1.



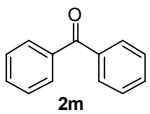
White solid; 73% yield (43.7 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.6 Hz, 2H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.3 Hz, 2H), 7.08 (d, *J* = 8.6 Hz, 2H), 2.57 (s, 3H), 2.45 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.6, 152.9, 145.8, 135.6, 132.0, 130.0, 129.9 128.4, 122.5, 26.6, 21.7.



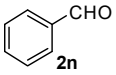
Colorless oil; 71% yield (26.7 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.4 Hz, 2H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.46 (t, *J* = 7.4 Hz, 2H), 3.26 (t, *J* = 10.8 Hz, 1H), 1.87 (t, *J* = 12.9 Hz, 4H), 1.74 (d, *J* = 11.9 Hz, 1H), 1.60–1.18 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.9, 136.3, 132.7, 128.6, 128.2, 45.6, 29.4, 25.9, 25.8.



Colorless oil; 62% yield (20.1 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.1 Hz, 2H), 7.50–7.34 (m, 3H), 1.35 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 209.2, 138.5, 130.7, 128.0, 127.7, 44.1, 28.9.

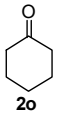


White solid; 70% yield (from **1m**, 26.4 mg); 69% yield (from **8f**, 25 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91–7.73 (m, 4H), 7.64–7.53 (m, 2H), 7.47 (t, *J* = 7.6 Hz, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.5, 137.4, 132.3, 129.9, 128.1.



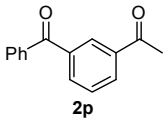
2n

Colorless oil; 81% yield (from **1n**, 34.0 mg); 62% yield (from **1o**, 13.2 mg); 33% yield (from **1p**, 7 mg); 80% yield (from **7e**, 18 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.01 (s, 1H), 7.87 (dd, *J* = 8.2, 1.2 Hz, 2H), 7.68–7.58 (m, 1H), 7.52 (t, *J* = 7.4 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 192.4, 136.3, 134.4, 129.7, 128.9.



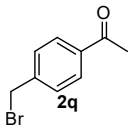
2o

Colorless oil; 68% yield (from **7b**, 13.4 mg); 71% yield (from **8k**, 14 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.29 (t, *J* = 6.4 Hz, 4H), 1.81 (d, *J* = 5.7 Hz, 4H), 1.69 (d, *J* = 4.1 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 212.1, 41.9, 26.9, 24.9.



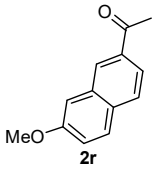
2p

White solid; 66% yield (29.5 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.36 (s, 1H), 8.17 (d, *J* = 7.8 Hz, 1H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.79 (d, *J* = 7.5 Hz, 2H), 7.68–7.54 (m, 2H), 7.50 (t, *J* = 7.5 Hz, 2H), 2.64 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.2, 195.8, 138.0, 137.1, 136.9, 134.2, 132.8, 131.7, 130.0, 129.6, 128.7, 128.4, 26.7.



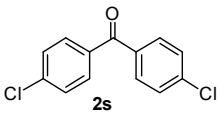
2q

White solid; 40% yield (17.0 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.1 Hz, 2H), 7.47 (d, *J* = 8.1 Hz, 2H), 4.49 (s, 2H), 2.59 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.4, 142.8, 136.8, 129.2, 128.8, 32.1, 26.7.



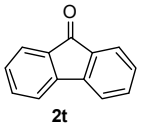
2r

White solid; 85% yield (34.0 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.38 (s, 1H), 8.00 (d, *J* = 8.6 Hz, 1H), 7.84 (d, *J* = 8.9 Hz, 1H), 7.76 (d, *J* = 8.6 Hz, 1H), 7.20 (d, *J* = 9.0 Hz, 1H), 7.14 (s, 1H), 3.94 (s, 3H), 2.69 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.8, 159.7, 137.2, 132.6, 131.1, 130.0, 127.8, 127.0, 124.6, 119.7, 105.7, 55.4, 26.5.



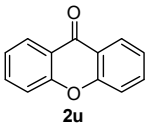
2s

White solid; 62% yield (31.0 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.6 Hz, 4H), 7.47 (d, *J* = 7.7 Hz, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 194.2, 139.1, 135.5, 131.3, 128.8.



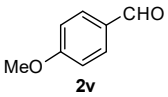
2t

White solid; 74% yield (26.8 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.3 Hz, 2H), 7.54–7.43 (m, 4H), 7.33–7.25 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 193.9, 144.4, 134.7, 134.1, 129.0, 124.3, 120.3.



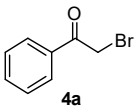
2u

White solid; 97% yield (38.0 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.34 (d, *J* = 7.9 Hz, 2H), 7.73 (t, *J* = 7.7 Hz, 2H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.38 (t, *J* = 7.5 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 177.2, 156.1, 134.8, 126.7, 123.9, 121.7, 117.9.



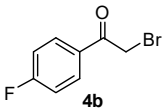
2v

Colorless oil; 73% yield (20.0 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.86 (s, 1H), 7.81 (d, *J* = 8.4 Hz, 2H), 6.98 (d, *J* = 8.3 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 190.8, 164.5, 131.9, 129.8, 114.2, 55.5.



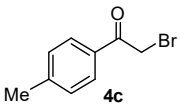
4a

White solid; 82% yield (28.7 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.02–7.94 (m, 2H), 7.65–7.56 (m, 1H), 7.48 (dd, *J* = 10.4, 4.7 Hz, 2H), 4.46 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 191.2, 133.9, 128.9, 128.8, 30.9.



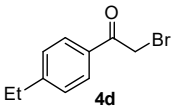
4b

White solid; 80% yield (34.8 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.08–7.97 (m, 2H), 7.22–7.11 (m, 2H), 4.41 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.8, 166.1 (d, *J* = 256.7 Hz), 131.7 (d, *J* = 9.5 Hz), 130.3 (d, *J* = 3.0 Hz), 116.1 (d, *J* = 22.1 Hz), 30.4.



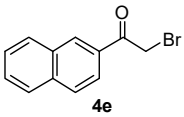
4c

White solid; 83% yield (35.3 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.3 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 4.43 (s, 2H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 191.0, 145.0, 131.4, 129.5, 129.0, 30.9, 21.8.



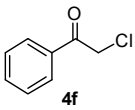
4d

White solid; 84% yield (38.3 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.3 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 4.44 (s, 2H), 2.72 (q, *J* = 7.6 Hz, 2H), 1.27 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 191.0, 151.1, 131.6, 129.2, 128.4, 31.0, 29.0, 15.1.



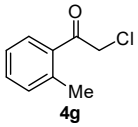
4e

White solid; 74% yield (36.8 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 (s, 1H), 7.99 (dd, *J* = 14.5, 8.3 Hz, 2H), 7.94–7.84 (m, 2H), 7.70–7.49 (m,2H), 4.58 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 191.2, 135.8, 132.3, 131.2, 130.9, 129.6, 129.0, 128.8, 127.8, 127.0, 124.1, 31.0.



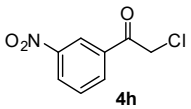
4f

White solid; 74% yield (22.9 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.3 Hz, 2H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 4.72 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 191.0, 134.2, 134.0, 128.9, 128.5, 46.0.



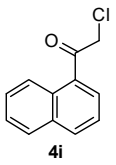
4g

White solid; 73% yield (23.4 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.0 Hz, 1H), 7.30 (d, *J* = 7.4 Hz, 2H), 4.64 (s, 2H), 2.53 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 194.2, 139.5, 134.5, 132.4, 128.6, 125.8, 47.9, 21.4.



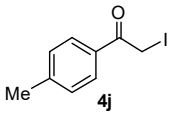
4h

White solid; 60% yield (23.9mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.79 (t, *J* = 1.9 Hz, 1H), 8.48 (ddd, *J* = 8.2, 2.1, 0.9 Hz, 1H), 8.39–8.24 (m, 1H), 7.74 (t, *J* = 8.0 Hz, 1H), 4.73 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.3, 148.5, 135.3, 134.1, 130.3 128.2, 123.5, 45.4.



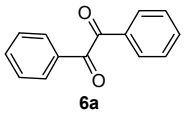
4i

White solid; 72% yield (23.2 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.63 (d, *J* = 8.5 Hz, 1H), 8.05 (d, *J* = 8.3 Hz, 1H), 7.89 (t, *J* = 7.4 Hz, 2H), 7.69–7.47 (m, 3H), 4.78 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 194.4, 134.0, 133.9, 132.4, 130.4, 128.6, 128.5, 128.2, 126.8, 125.5, 124.2, 48.0.



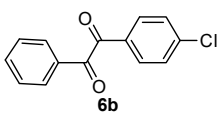
4j

White solid; 63% yield (30.9 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.6 Hz, 2H), 7.29 (d, *J* = 7.7 Hz, 2H), 4.70 (s, 2H), 2.42 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 190.7, 145.1, 131.7, 129.6, 128.6, 46.0, 21.8.



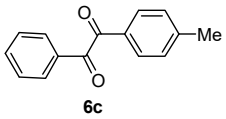
6a

Yellow solid; 77% yield (32.4 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.7 Hz, 4H), 7.66 (t, *J* = 7.3 Hz, 2H), 7.51 (t, *J* = 7.5 Hz, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 194.6, 134.9, 132.9, 129.9, 129.0.



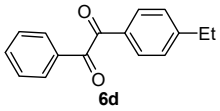
6b

Yellow solid; 70% yield (34.3 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 11.5, 8.6 Hz, 4H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.51 (dd, *J* = 12.3, 7.9 Hz, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 193.9, 193.1, 141.6, 135.1, 132.8, 131.3, 131.2, 129.9, 129.4, 129.1.



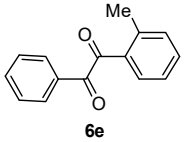
6c

Yellow solid; 68% yield (30.5 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.8 Hz, 2H), 7.87 (d, *J* = 7.7 Hz, 2H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.4 Hz, 2H), 7.31 (d, *J* = 7.7 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 194.8, 194.3, 146.3, 134.8, 132.9, 130.4, 130.0, 129.9, 129.7, 129.0, 22.0.



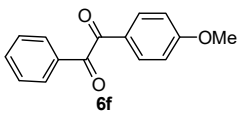
6d

Yellow solid; 56% yield (26.7 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.8 Hz, 2H), 7.89 (d, *J* = 7.8 Hz, 2H), 7.65 (t, *J* = 7.0 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 2H), 7.33 (d, *J* = 7.9 Hz, 2H), 2.72 (q, *J* = 7.6 Hz, 2H), 1.25 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 194.8, 194.4, 152.4, 134.8, 132.9, 130.6, 130.1, 129.9, 129.0, 128.6, 29.2, 15.1.



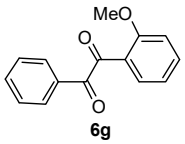
6e

Yellow solid; 73% yield (32.7 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.5 Hz, 2H), 7.62 (t, *J* = 7.6 Hz, 2H), 7.47 (dd, *J* = 14.5, 7.2 Hz, 3H), 7.31 (d, *J* = 7.5 Hz, 1H), 7.23 (s, 1H), 2.68 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.8, 194.8, 141.4, 134.7, 133.8, 133.1, 133.0, 132.6, 131.8, 129.9, 129.0, 126.0, 21.9.



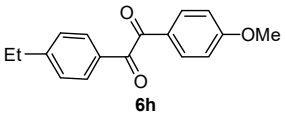
6f

Yellow oil; 70% yield (33.6 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.96 (t, *J* = 7.2 Hz, 4H), 7.65 (t, *J* = 7.3 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 2H), 6.97 (d, *J* = 8.5 Hz, 2H), 3.88 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 194.9, 193.2, 164.9, 134.8, 133.0, 132.4, 129.9, 128.9, 125.9, 114.3, 55.6.



6g

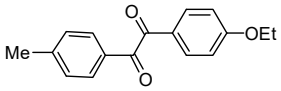
Yellow solid; 71% yield (34.1 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.7 Hz, 1H), 7.92 (d, *J* = 7.6 Hz, 2H), 7.61 (d, *J* = 6.1 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 2H), 7.13 (t, *J* = 7.5 Hz, 1H), 6.94 (d, *J* = 8.4 Hz, 1H), 3.56 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 194.7, 193.5, 160.4, 136.5, 133.8, 132.8, 130.5, 129.3, 128.7, 123.6, 121.5, 112.3, 55.6.



6h

Yellow solid; 73% yield (39.2 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 (dd, *J* = 15.9, 8.1 Hz, 4H), 7.32 (d, *J* = 7.9 Hz, 2H), 6.97 (d, *J* = 8.3 Hz, 2H), 3.88 (s, 3H), 2.72 (q, *J* = 7.5 Hz, 2H), 1.25 (t, *J* = 7.5 Hz, 3H); ^{13}C

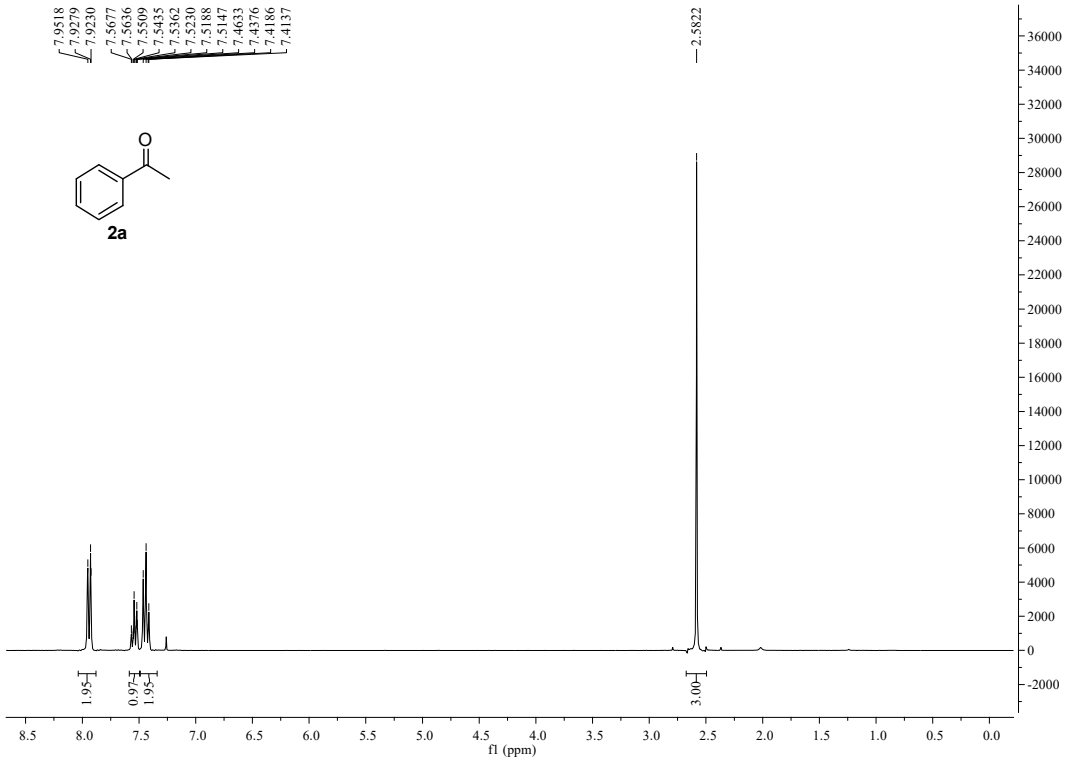
NMR (75 MHz, $CDCl_3$) δ 194.7, 193.4, 164.8, 152.1, 132.4, 130.8, 130.1, 128.5, 126.1, 114.3, 55.6, 29.1, 15.1.

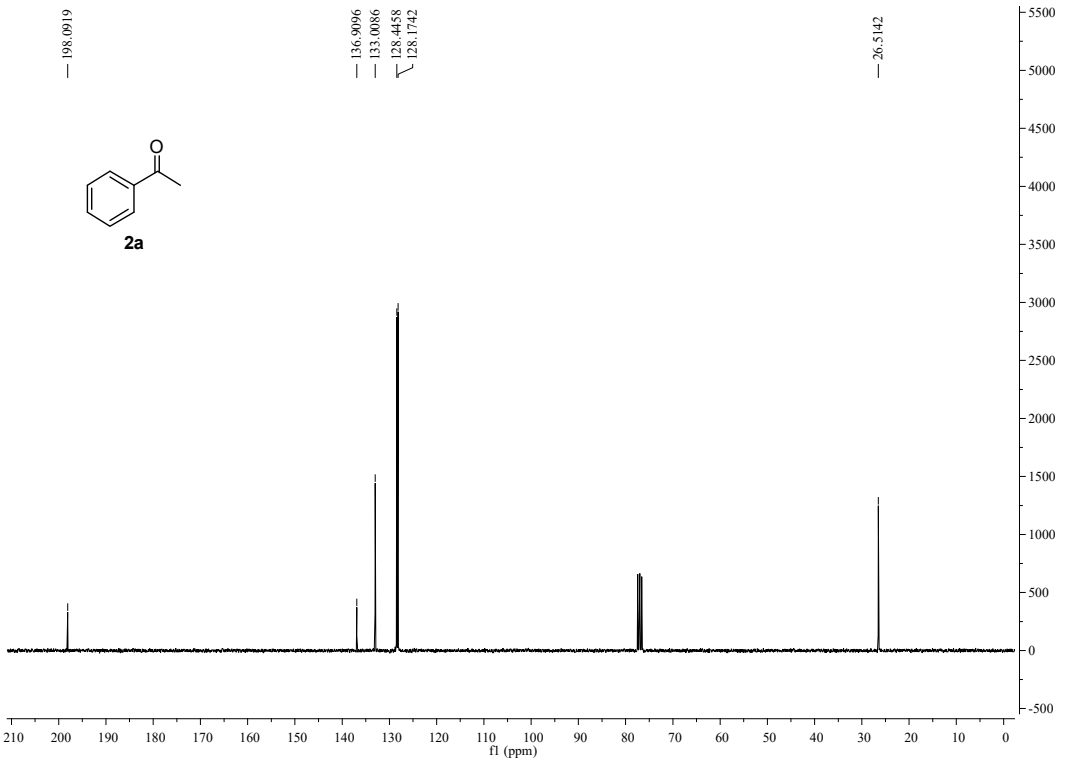


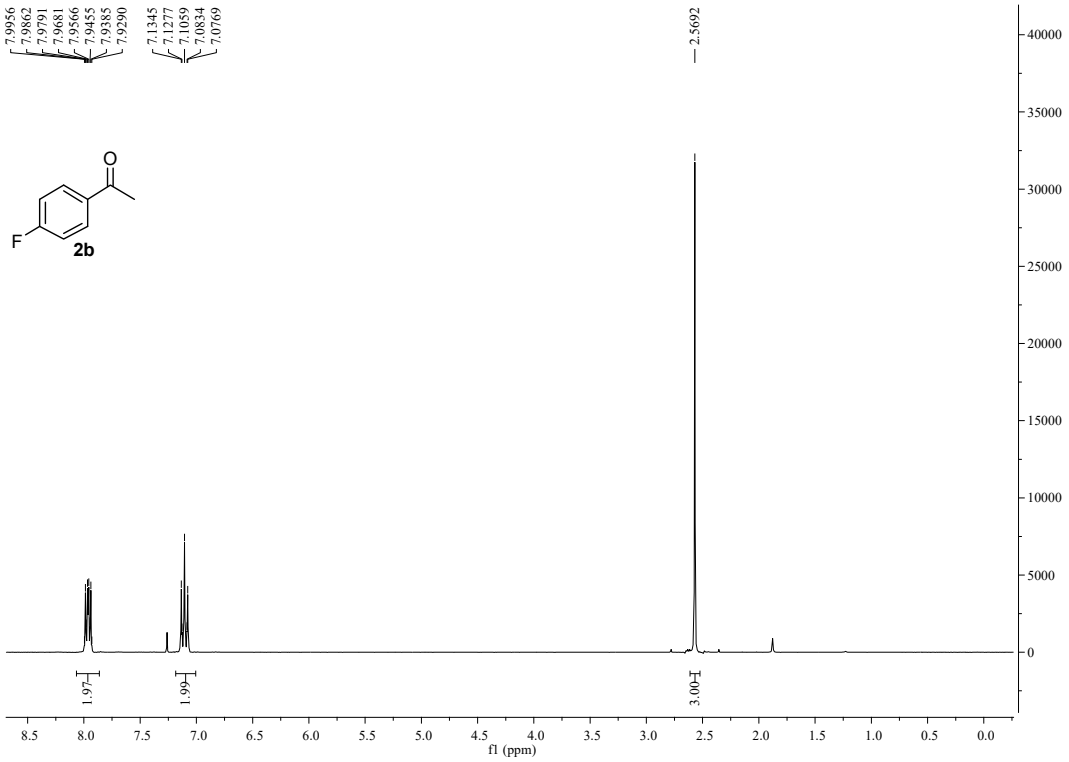
6i

Yellow solid; 61% yield (32.7 mg); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 18.1, 7.9 Hz, 4H), 7.29 (d, *J* = 7.7 Hz, 2H), 6.94 (d, *J* = 8.3 Hz, 2H), 4.11 (q, *J* = 6.7 Hz, 2H), 2.43 (s, 3H), 1.44 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 194.7, 193.4, 164.3, 146.0, 132.4, 130.8, 130.0, 129.6, 126.0, 114.7, 64.0, 21.9, 14.6.

10. ^{1}H and ^{13}C NMR spectra of products



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7.9566
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7.9385
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7.1345
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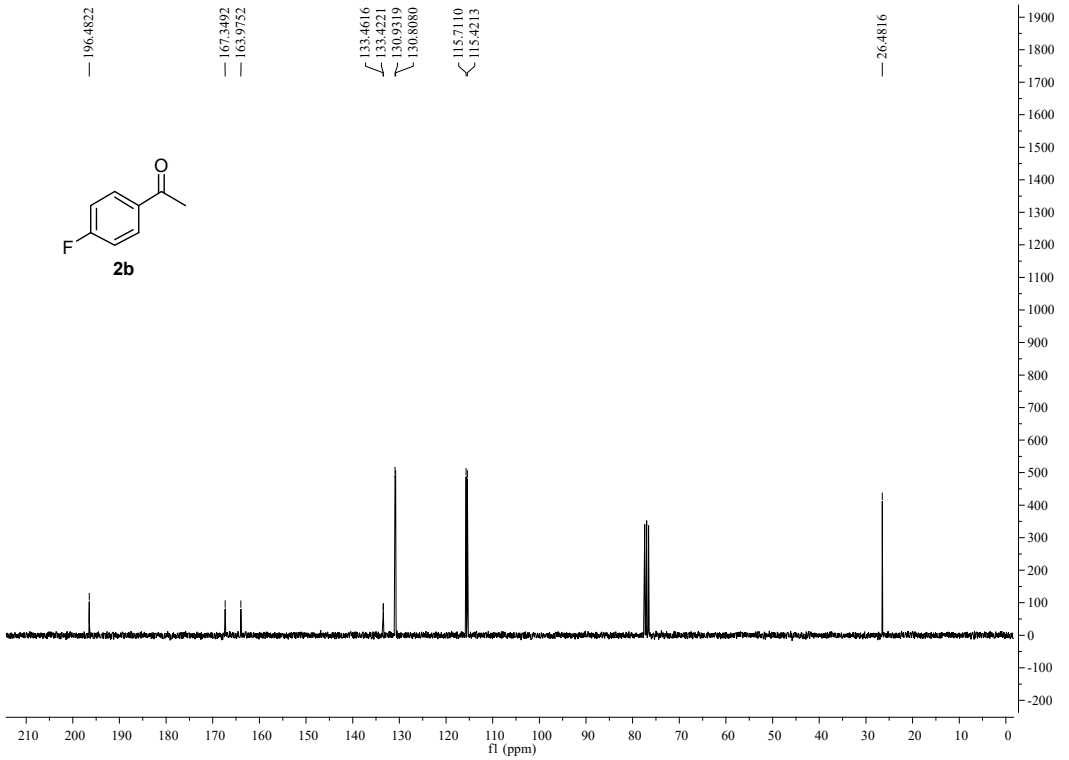
7.1059
7.0834
7.0769
2.5692
O
F
2b
1.97
1.99
3.00
f1 (ppm)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130.8080
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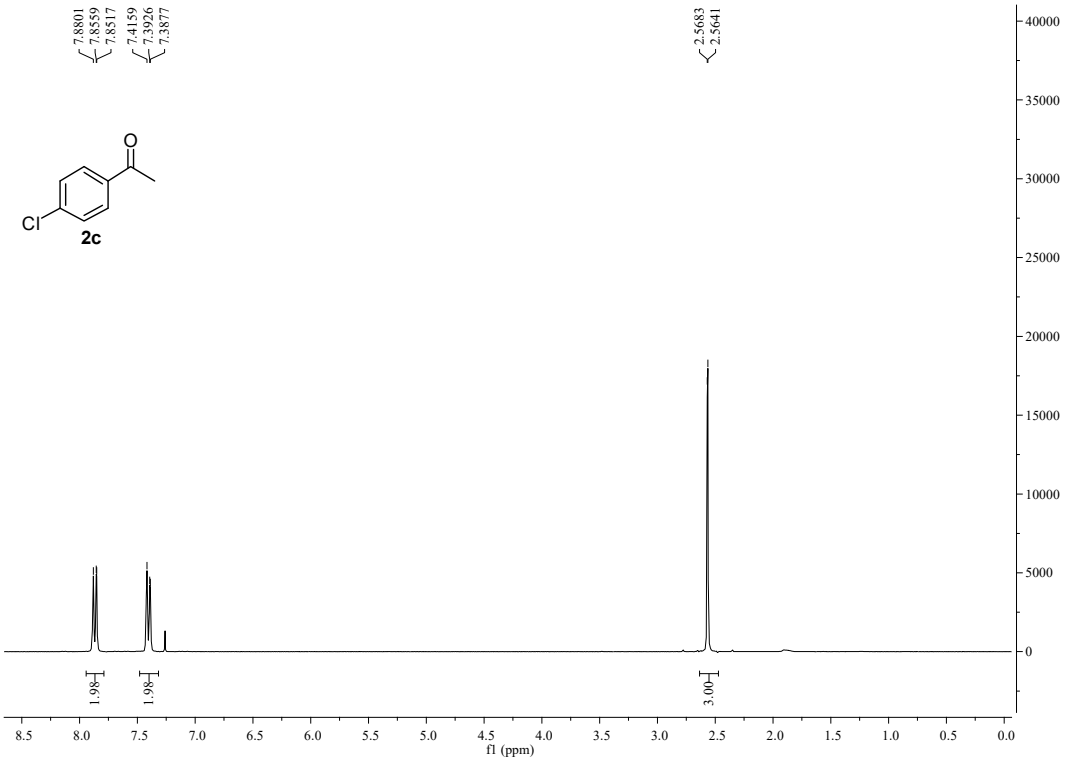
O
F
2b
f1 (ppm)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O
Cl
2c
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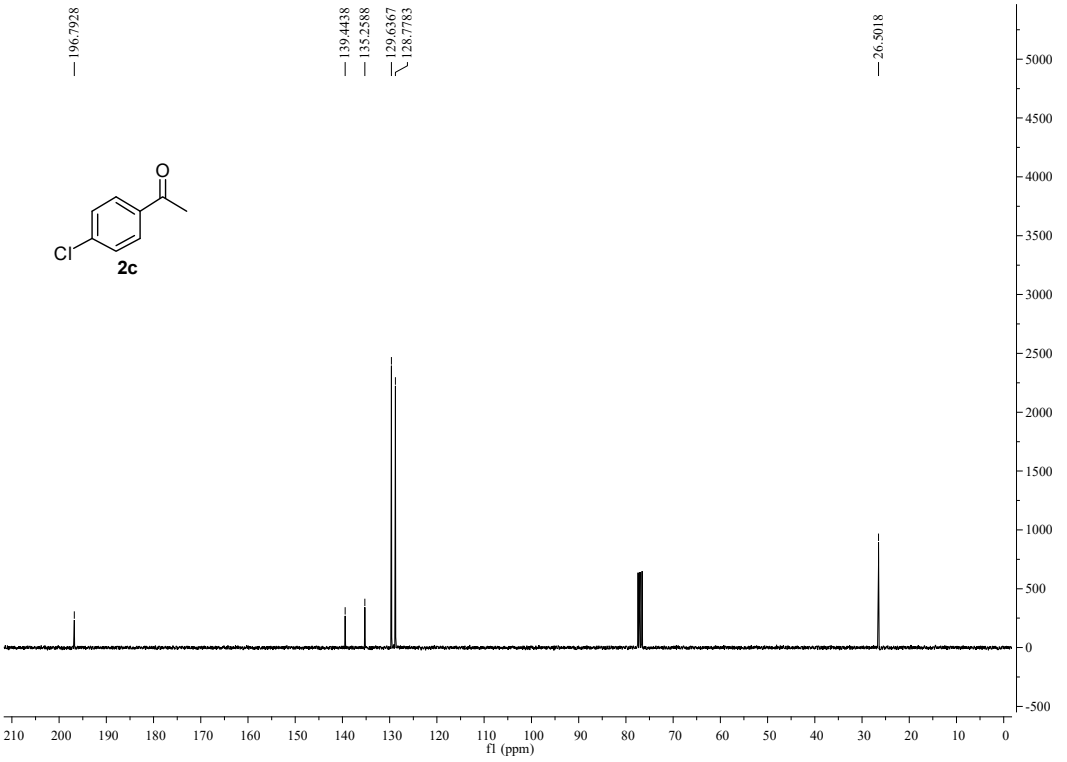
1.98
3.00
f1 (ppm)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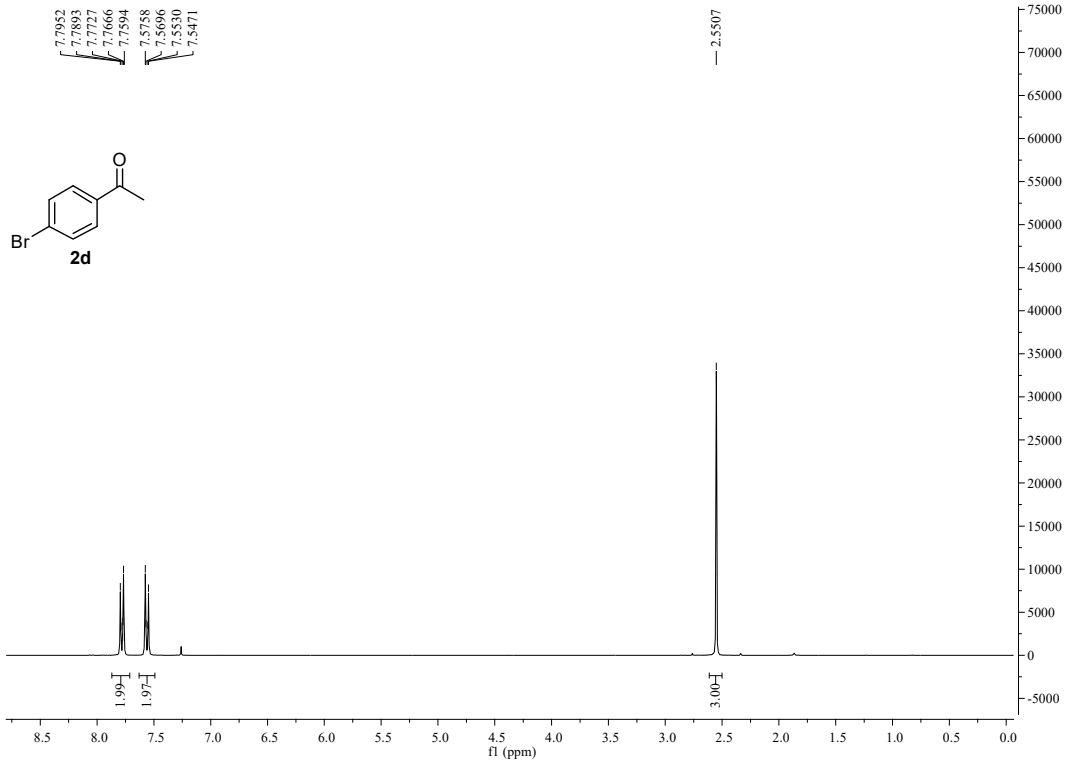
f1 (ppm)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2d
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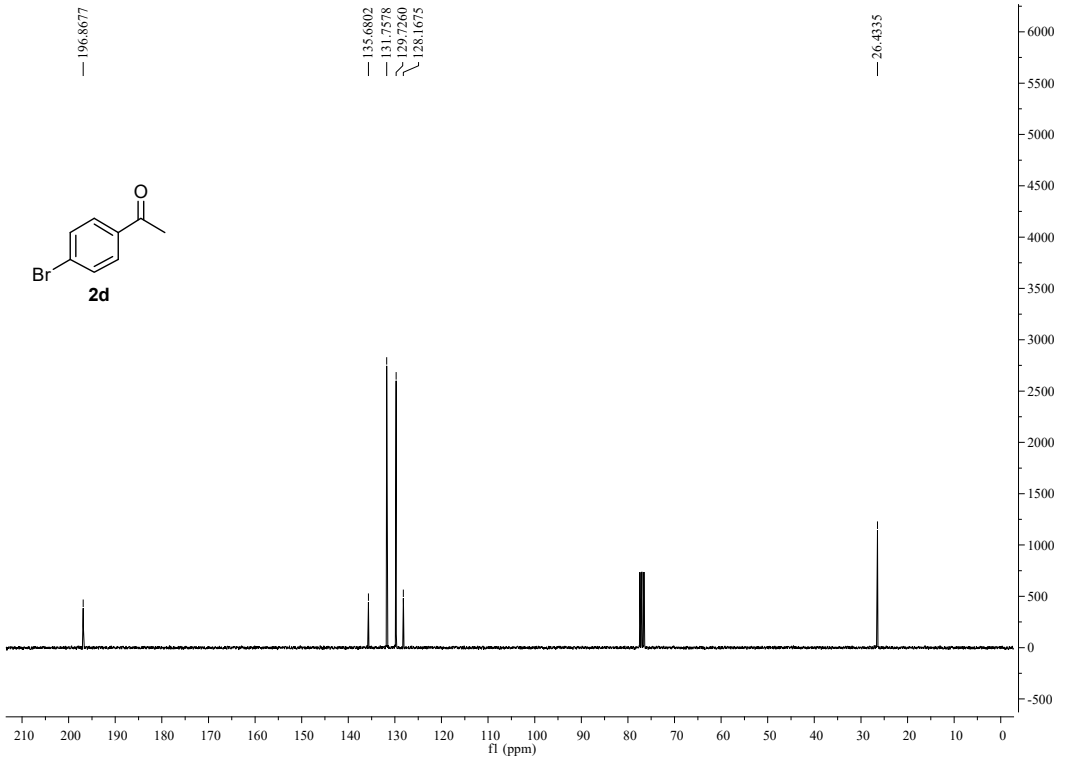
3.00
f1 (ppm)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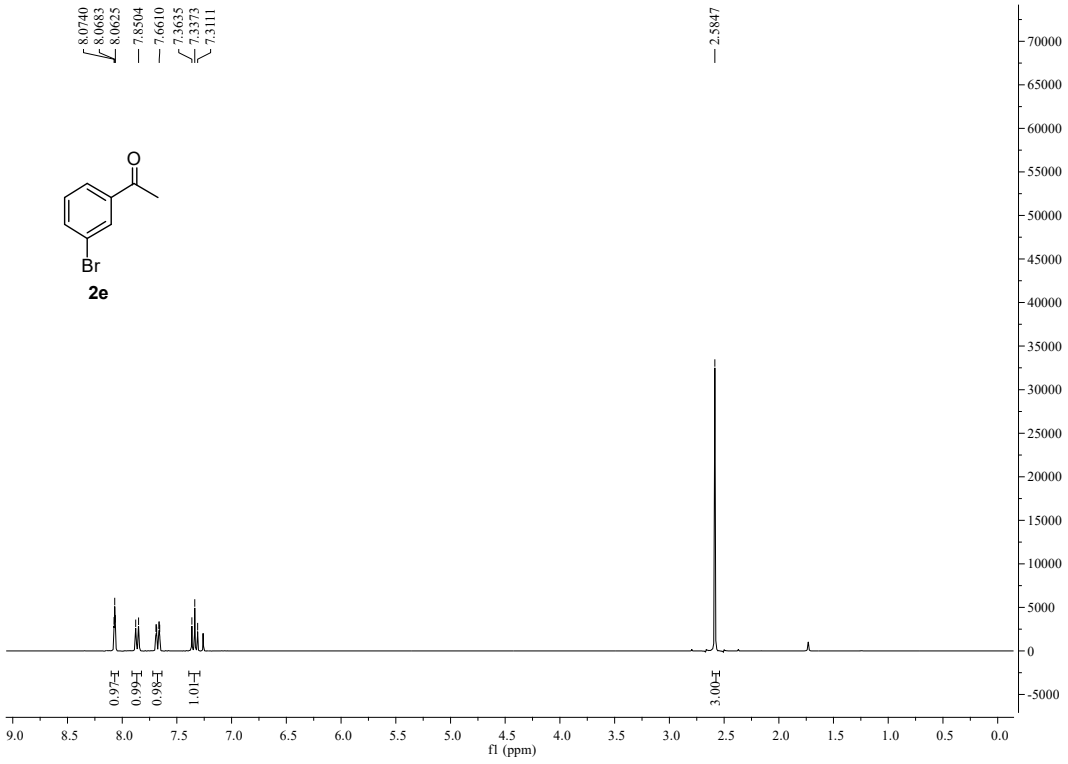
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2e
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0.98
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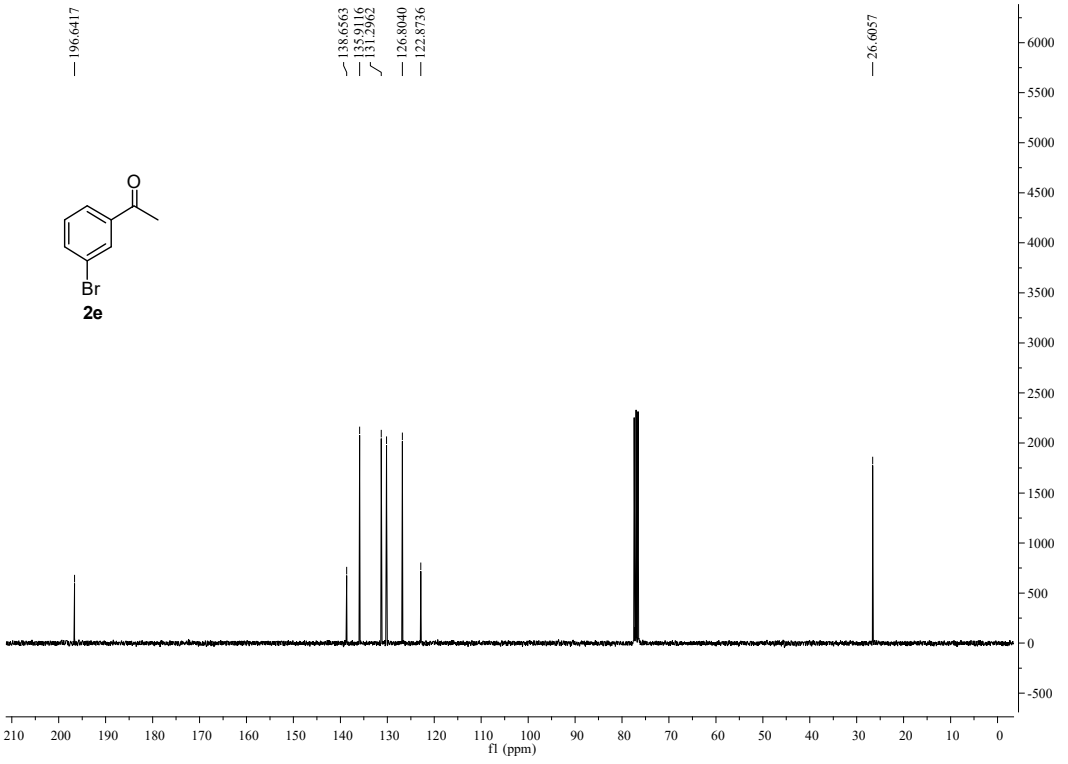
3.00
f1 (ppm)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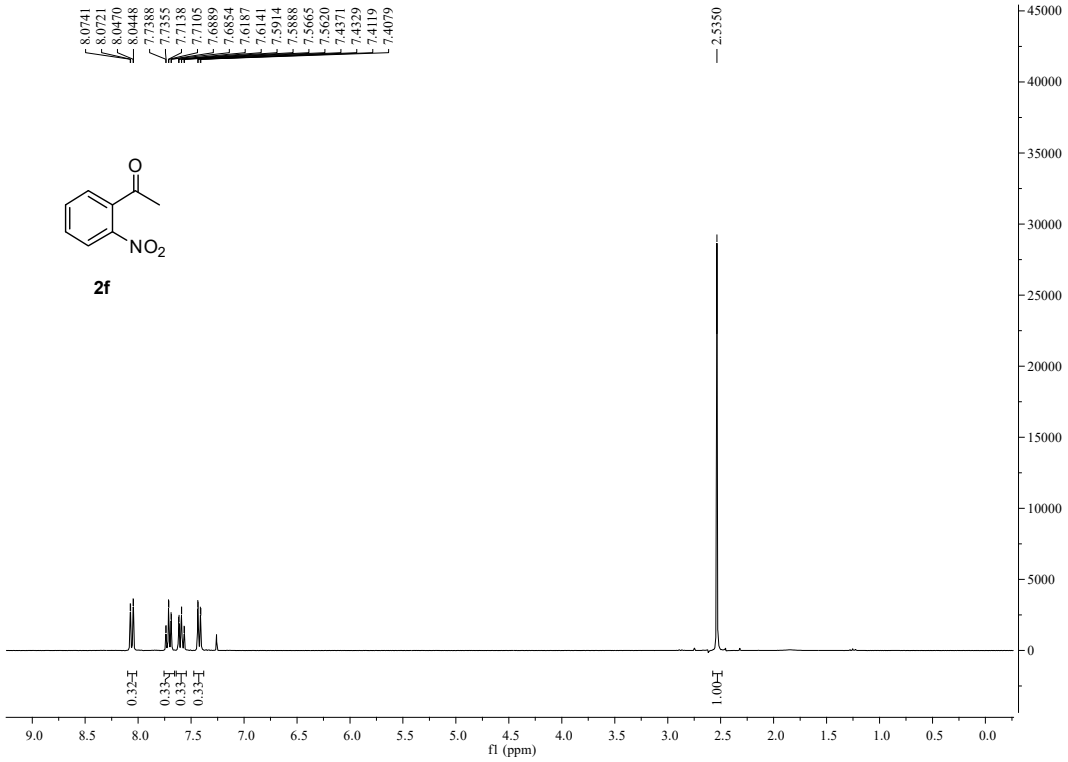
Br
2e
f1 (ppm)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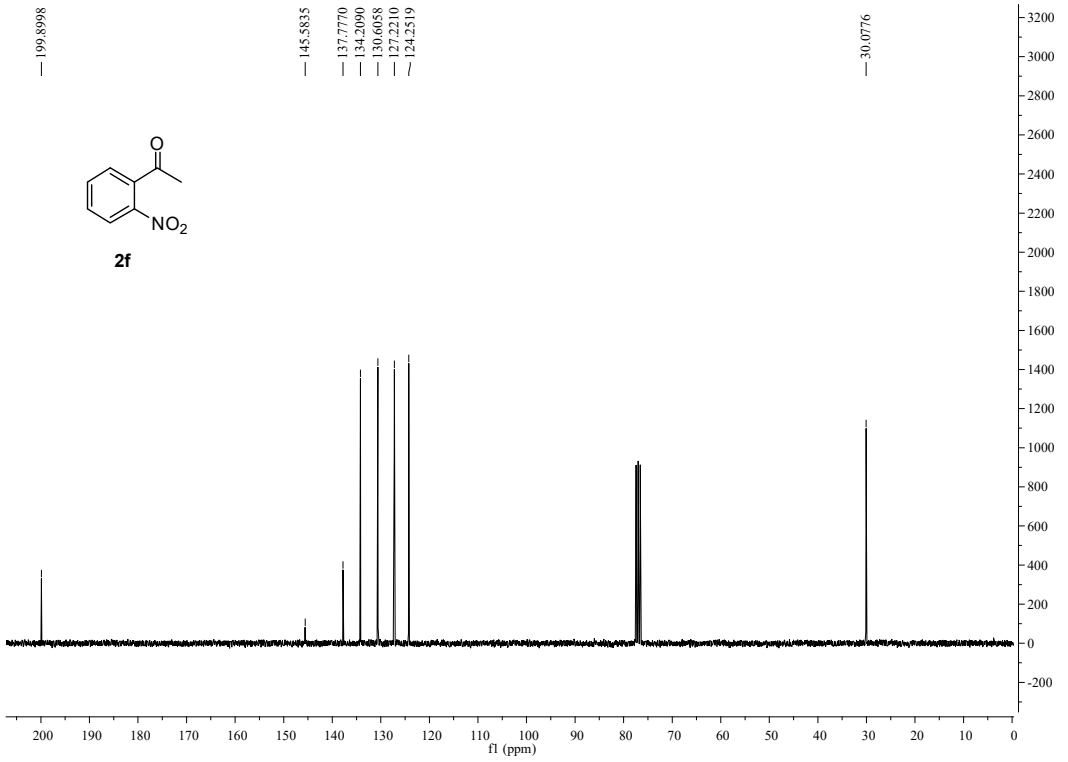
f1 (ppm)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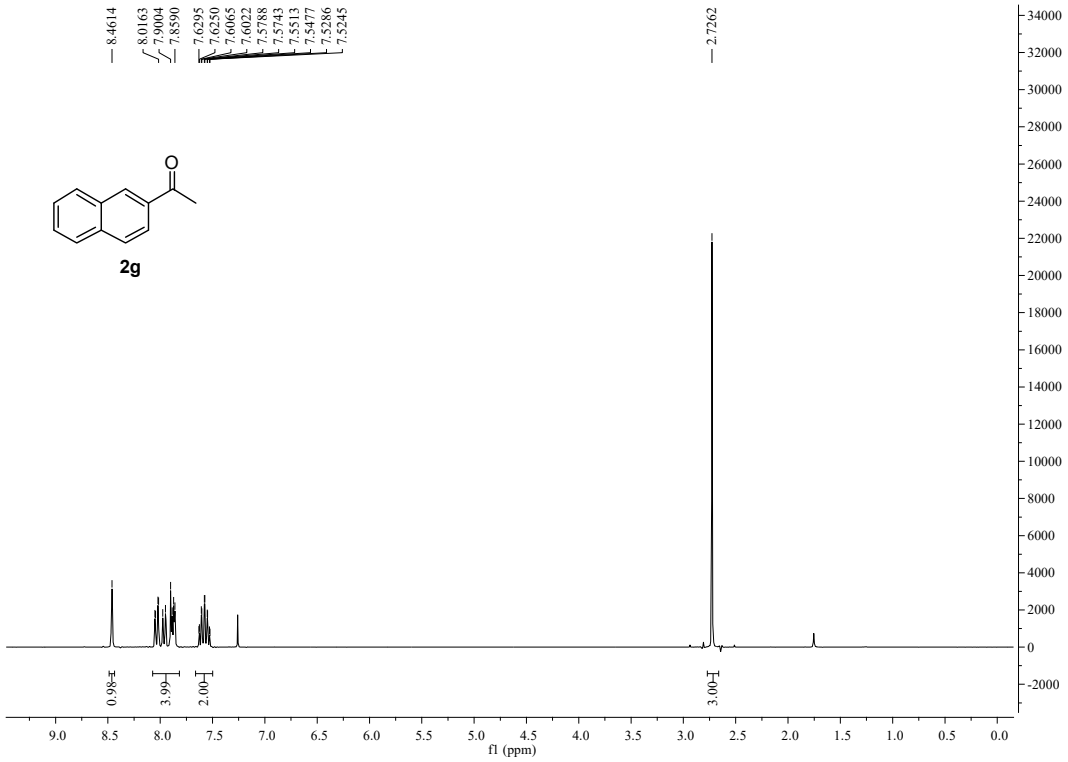
NO2
2f
f1 (ppm)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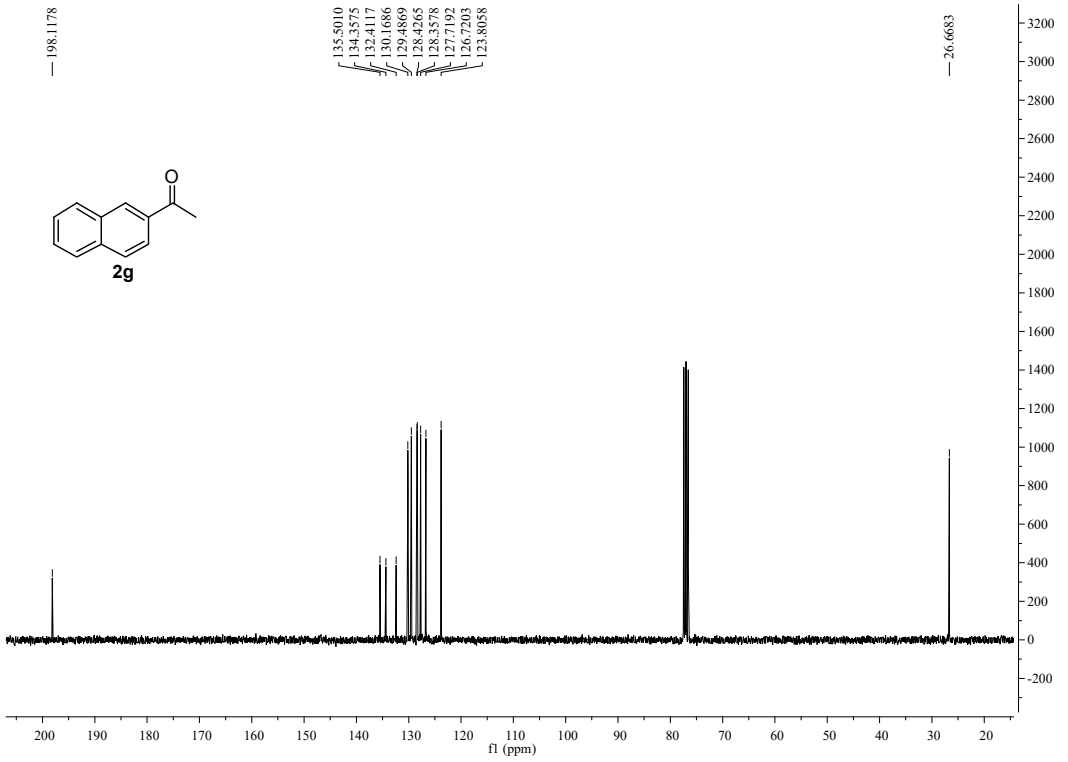
f1 (ppm)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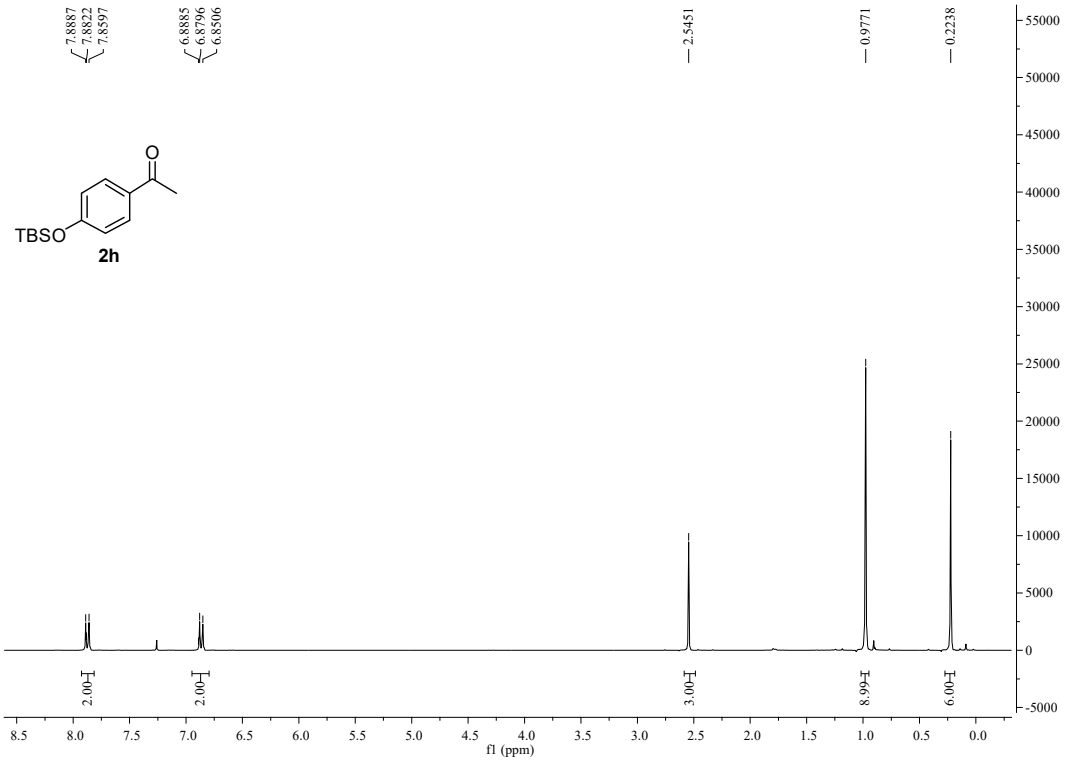
O
2g
f1 (ppm)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2h
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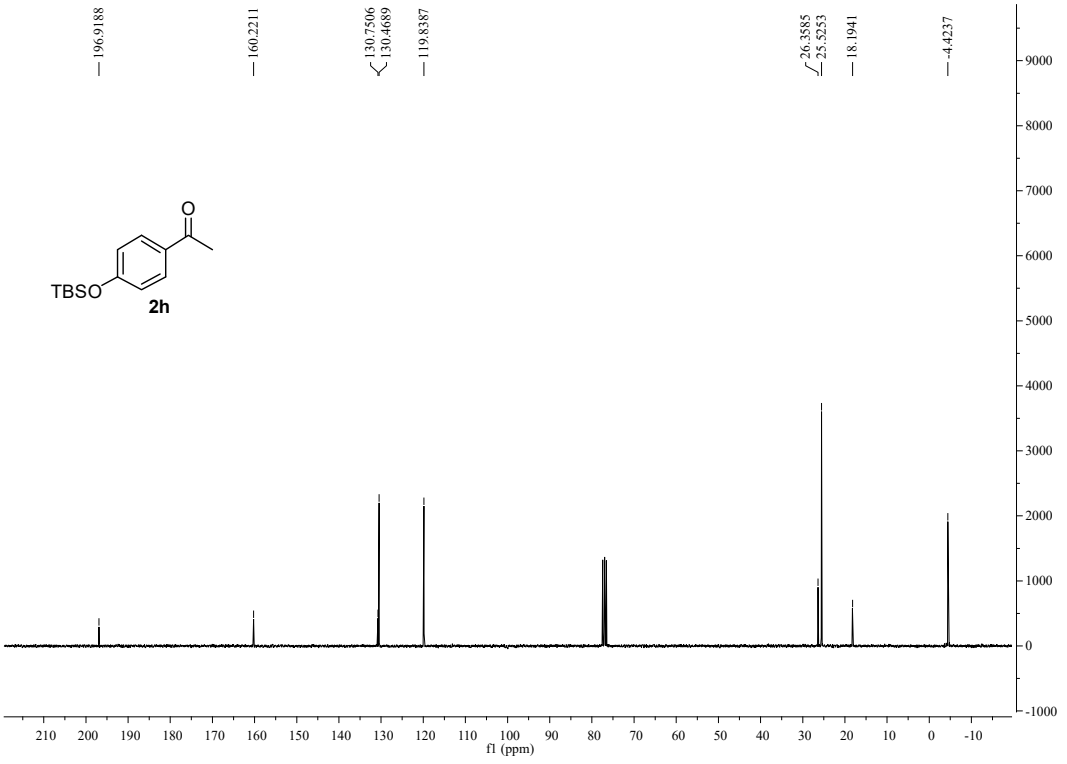
2.00
3.00
8.99
6.00
f1 (ppm)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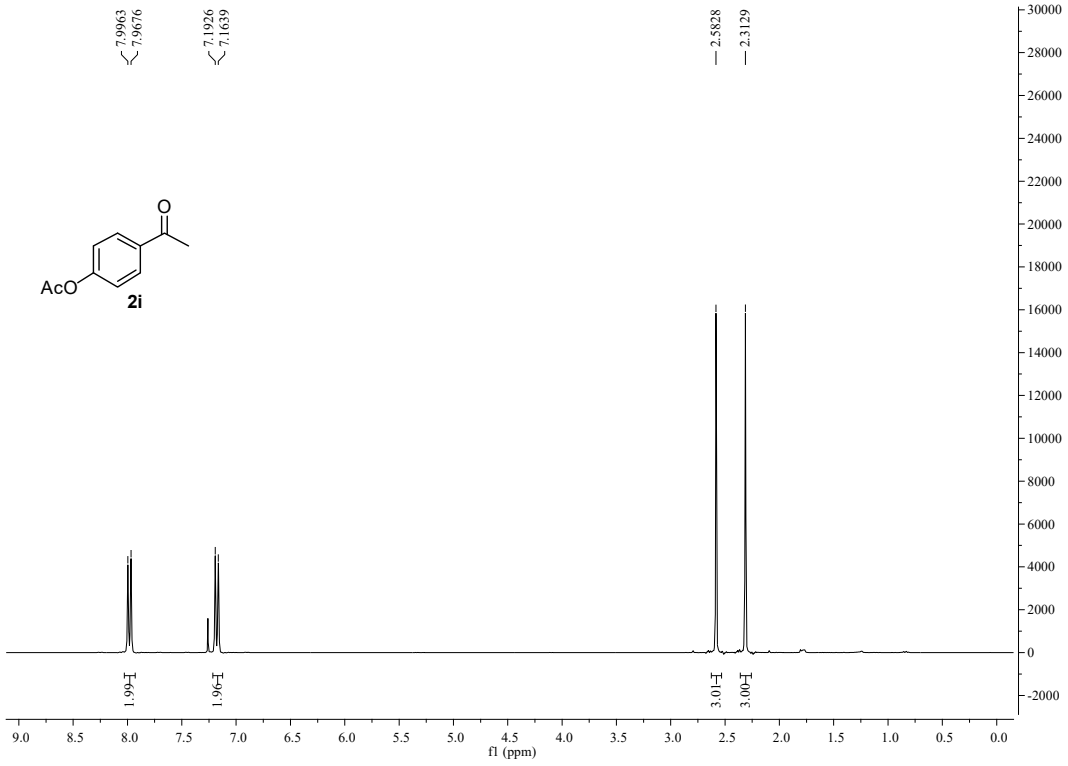
f1 (ppm)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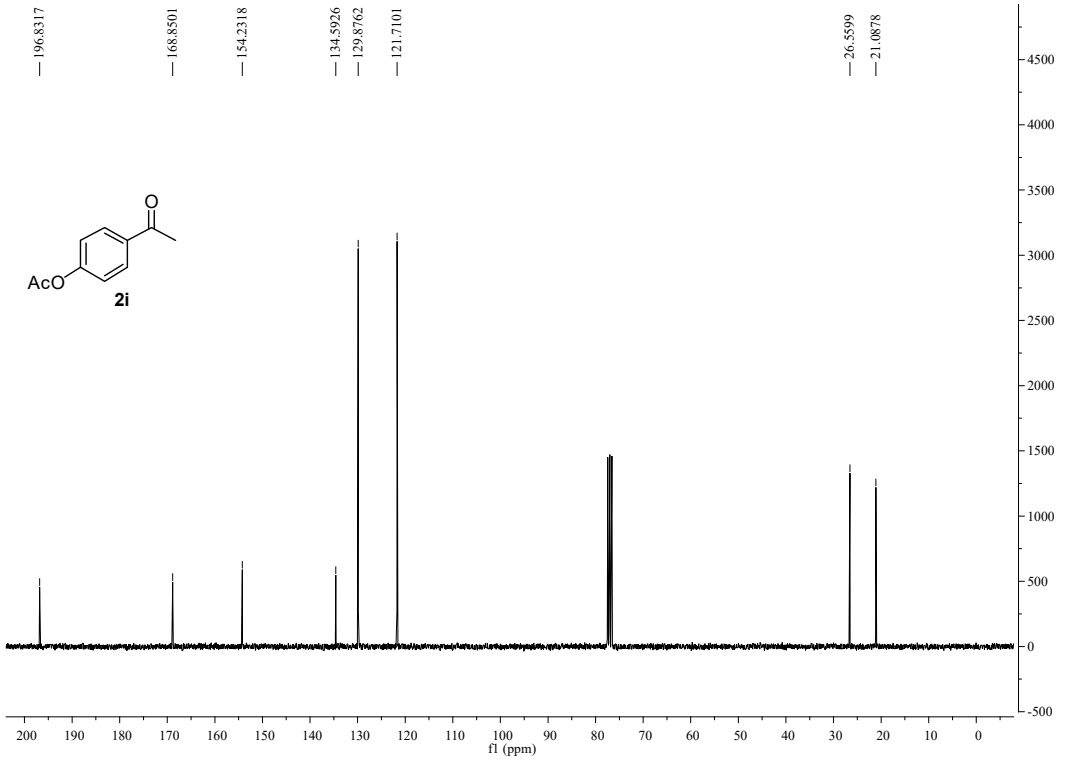
3.00
f1 (ppm)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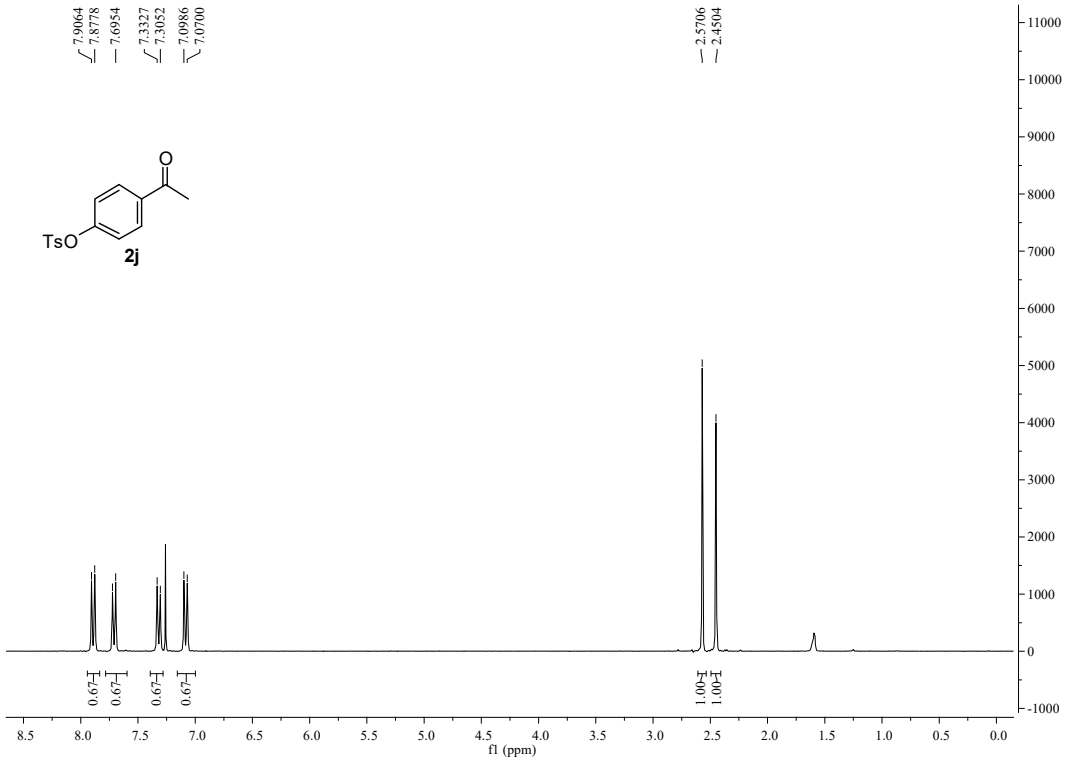
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0.67
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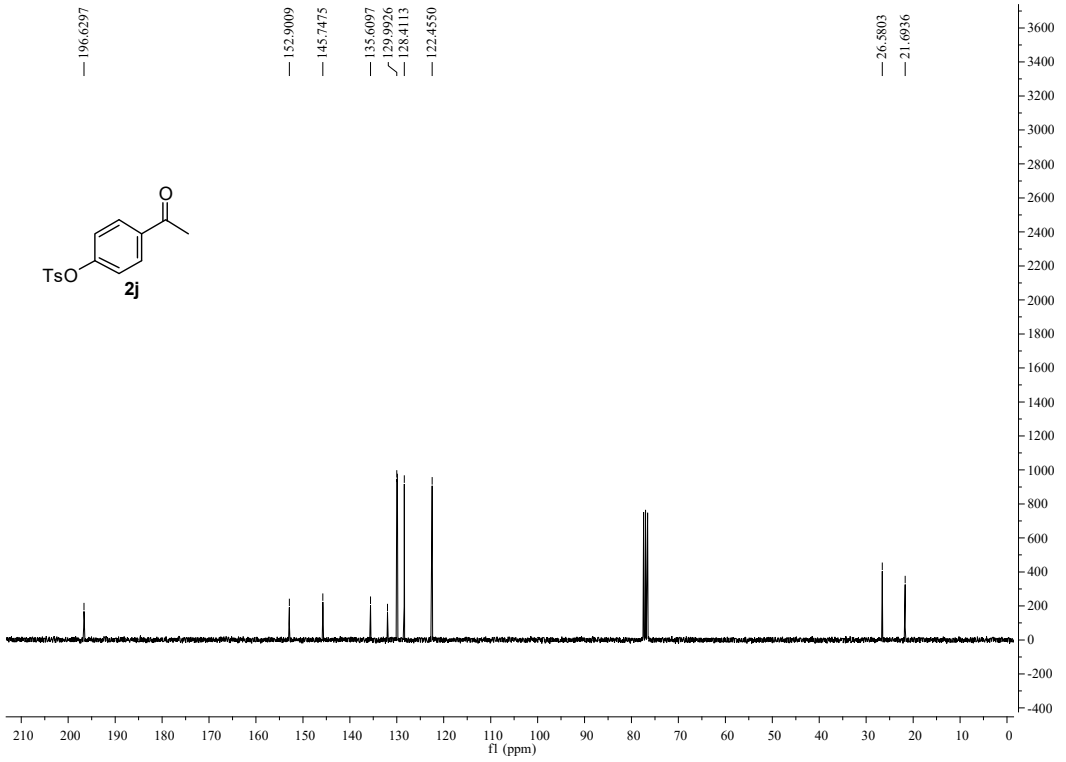
1.00
f1 (ppm)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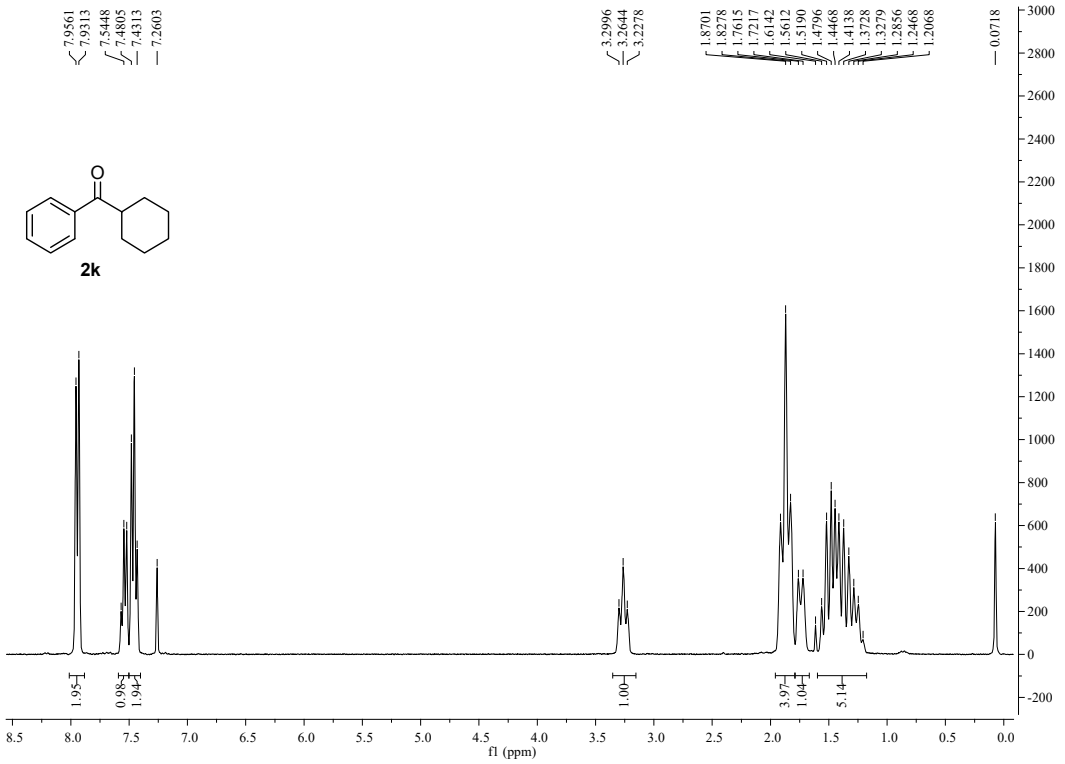
2j
f1 (ppm)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1.4138
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1.3279
1.2856
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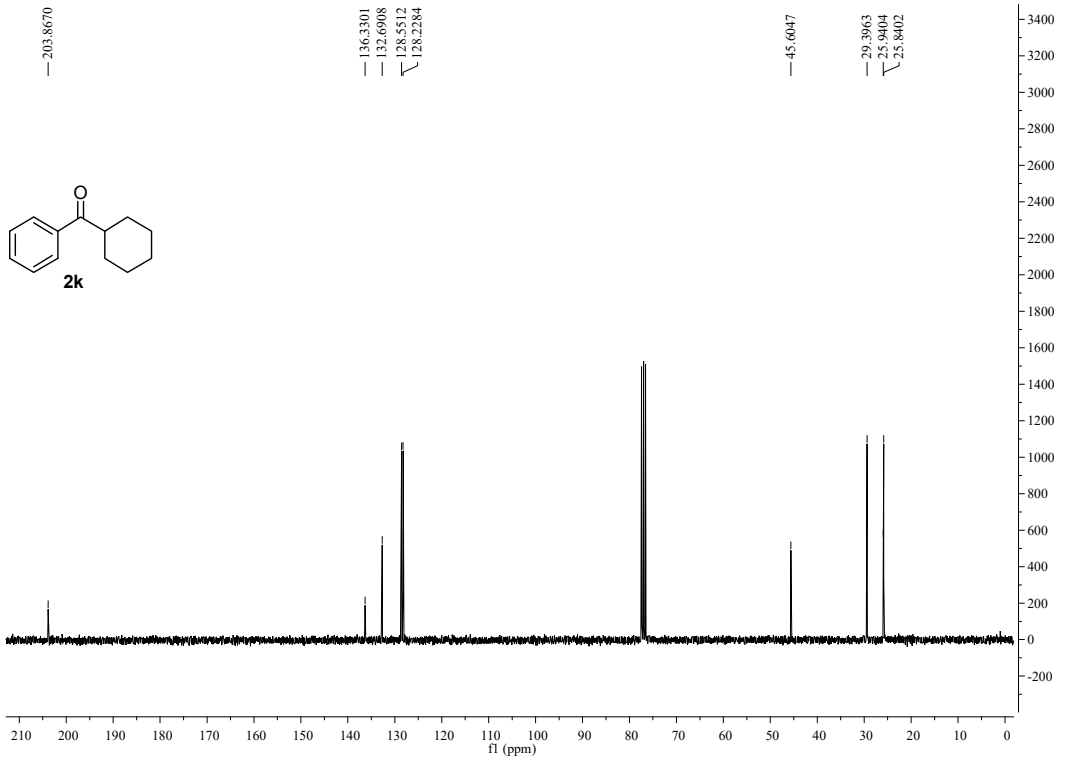
fl (ppm)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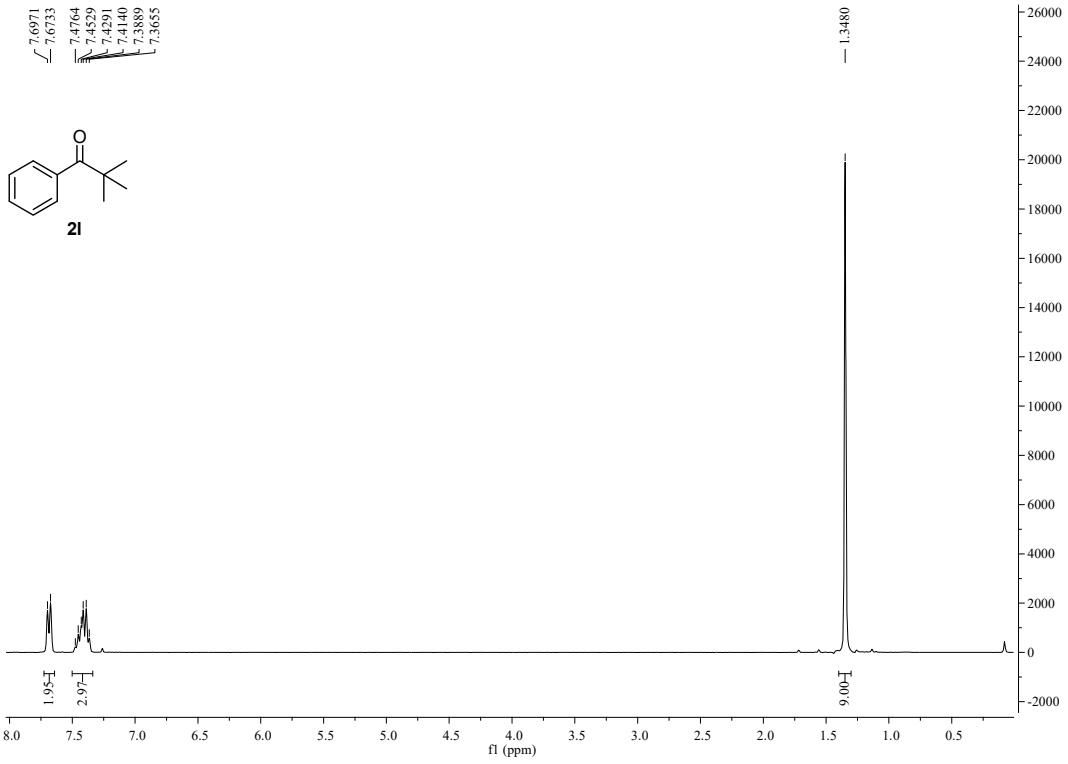
O
2k
fl (ppm)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2l
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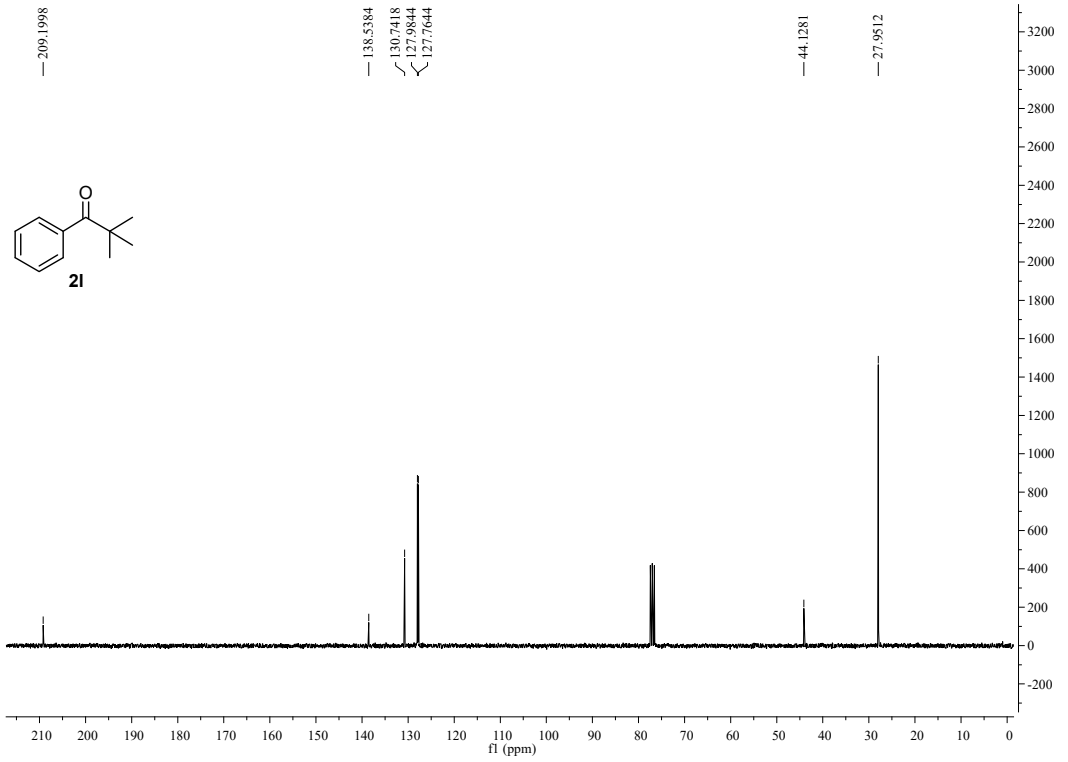
2.97
9.00
f1 (ppm)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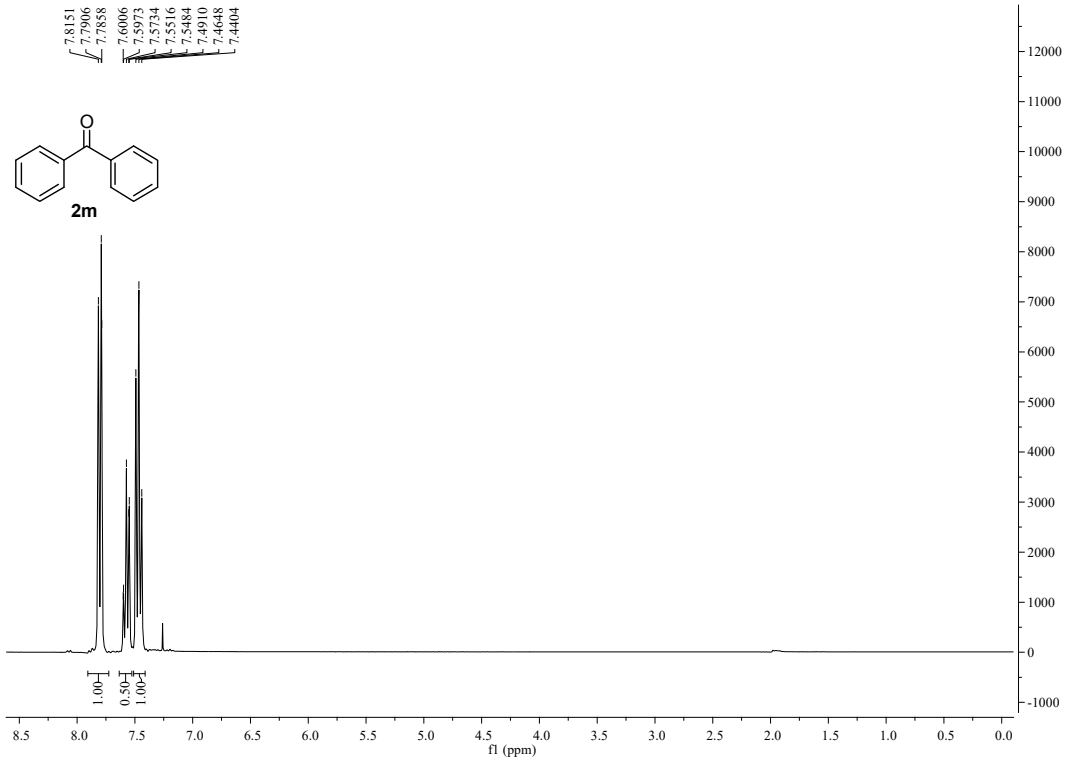
130.7418
127.9844
127.7644
44.1281
27.9512
2l
f1 (ppm)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7.7906
7.7858
7.6006
7.5973
7.5734
7.5516
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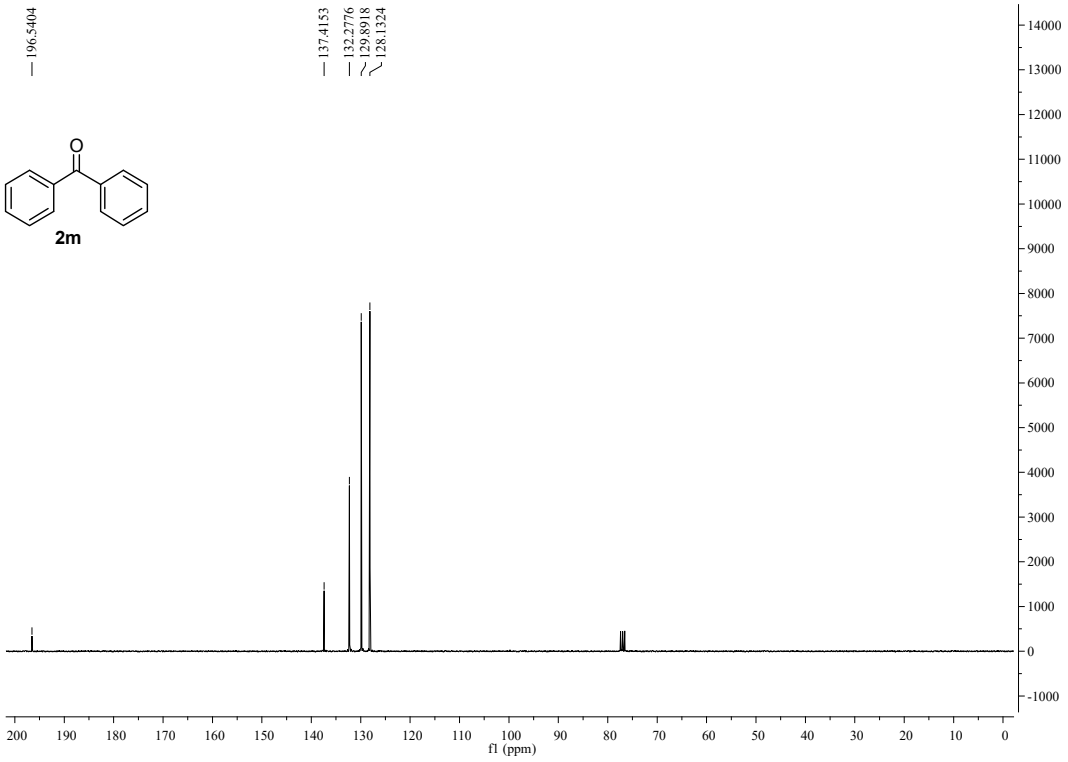
7.4910
7.4648
7.4404
O
2m
1.00
0.50
1.00
f1 (ppm)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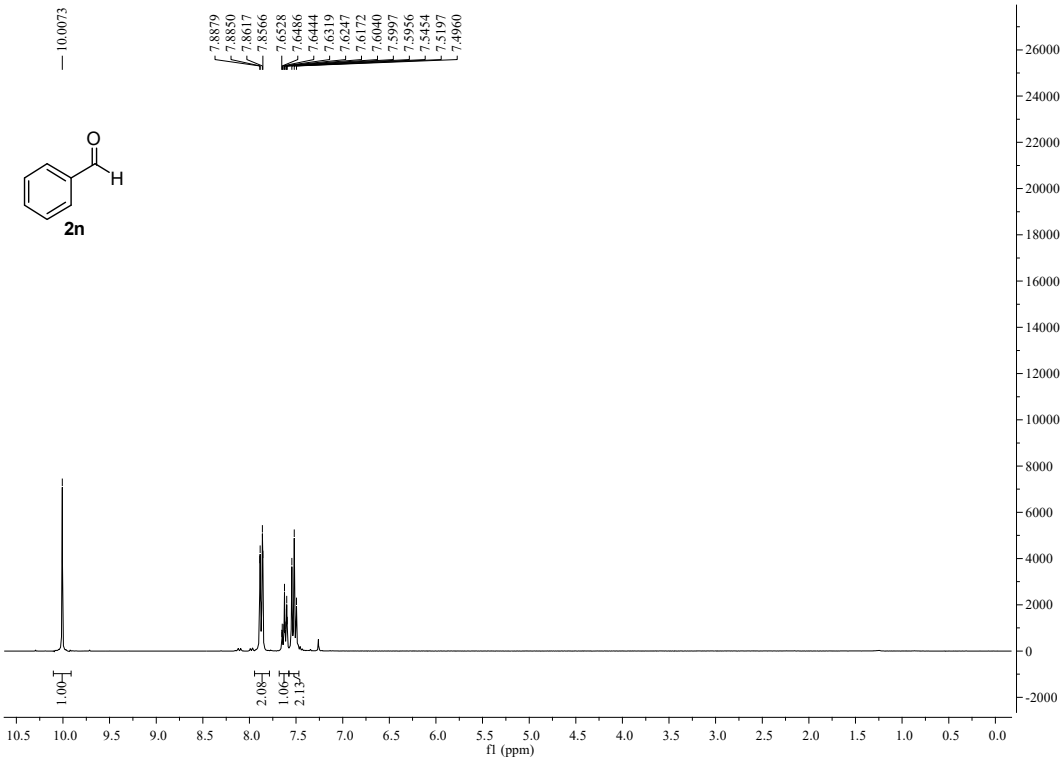
137.4153
132.2776
129.8918
128.1324
O
2m
f1 (ppm)


10.0073
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7.8850
7.8617
7.8566
7.6528
7.6486
7.6444
7.6319
7.6247
7.6172
7.6040
7.5997
7.5956
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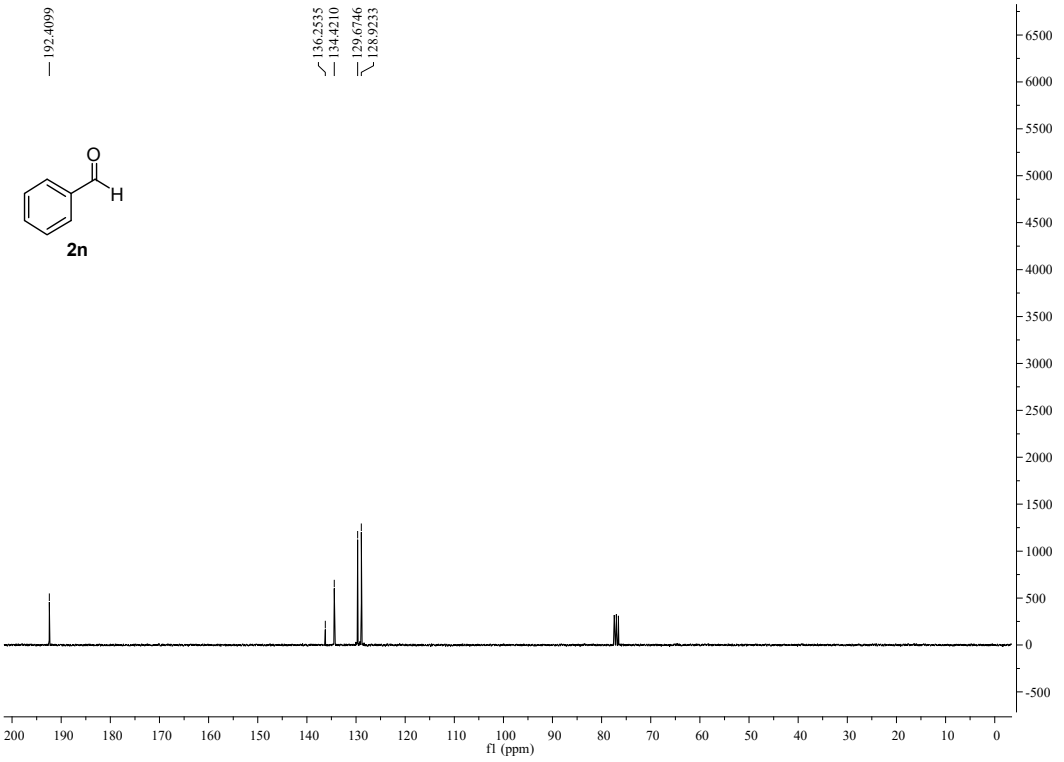
7.5197
7.4960
O
H
2n
1.00
2.08
1.06
2.13
f1 (ppm)


192.4099
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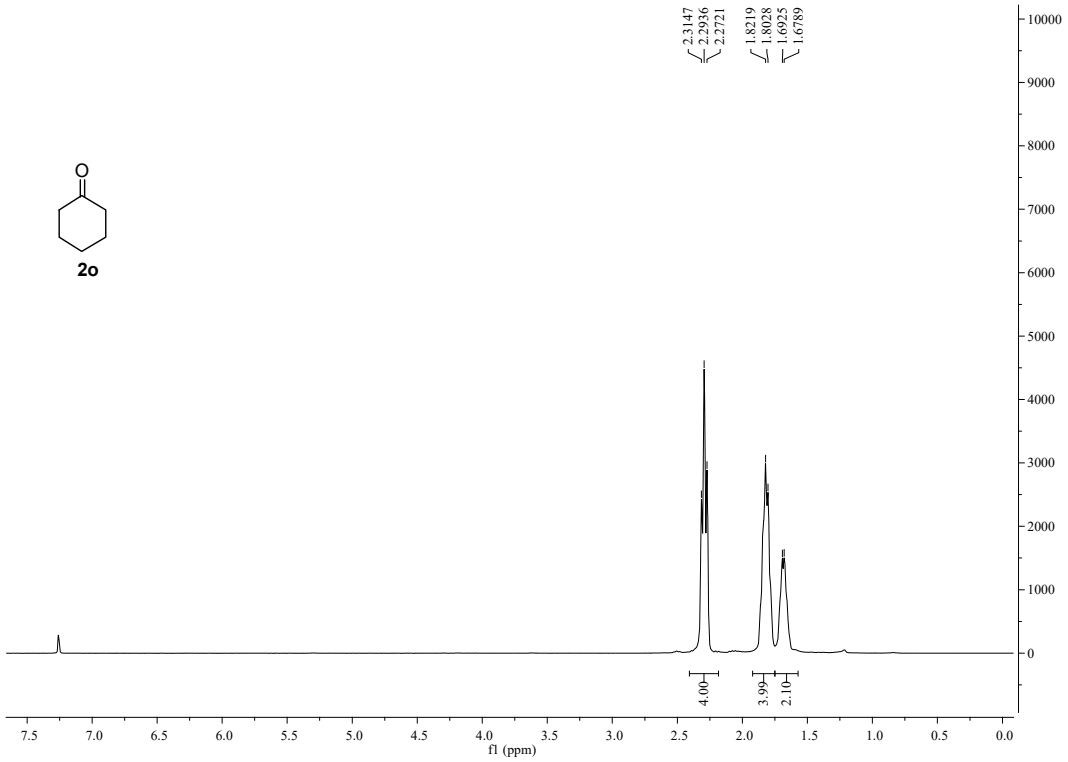
129.6746
128.9233
O
H
2n
f1 (ppm)


2.3147
2.2936
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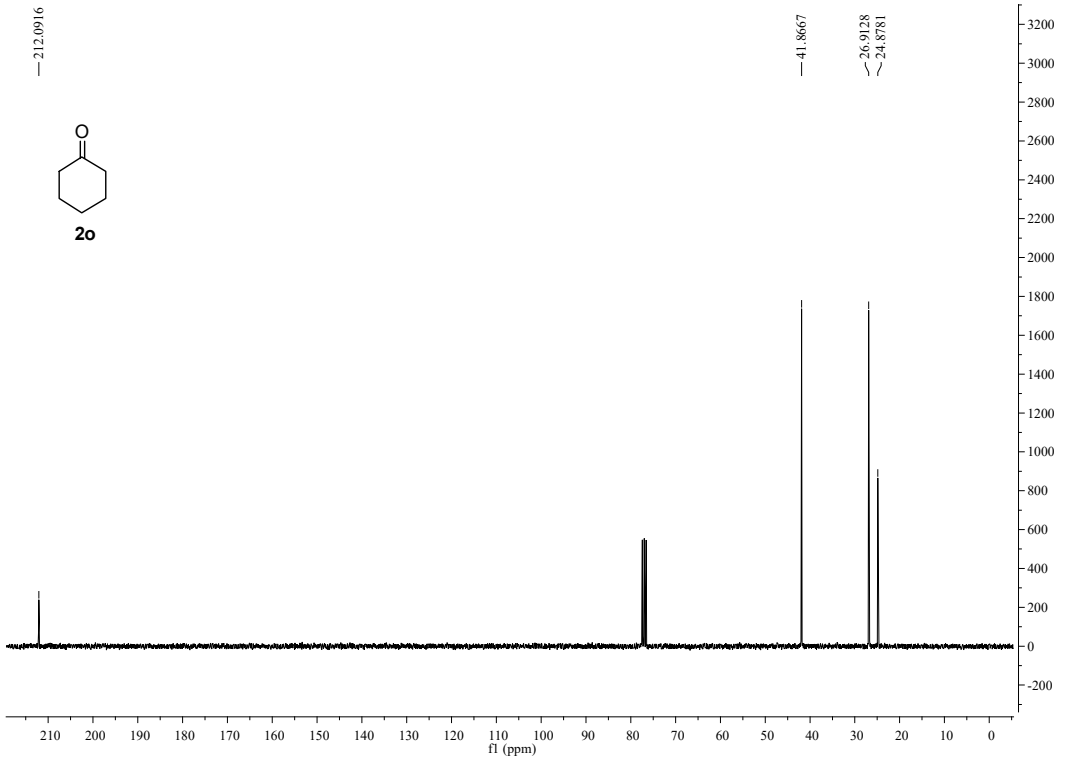
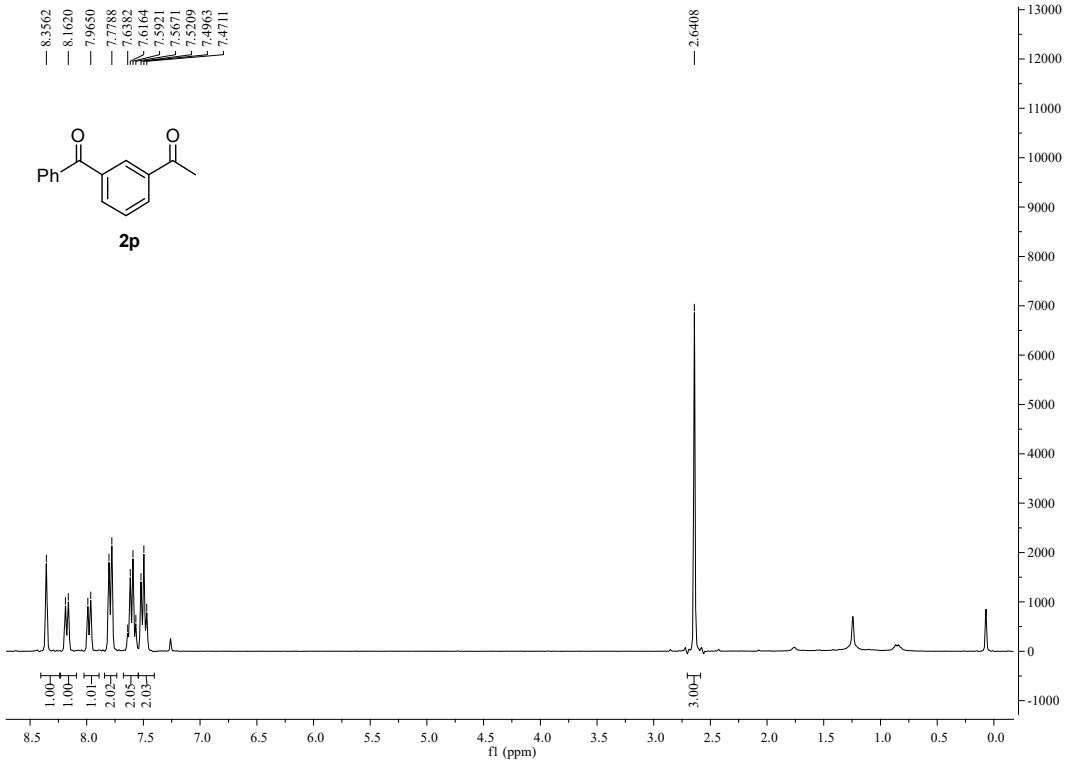
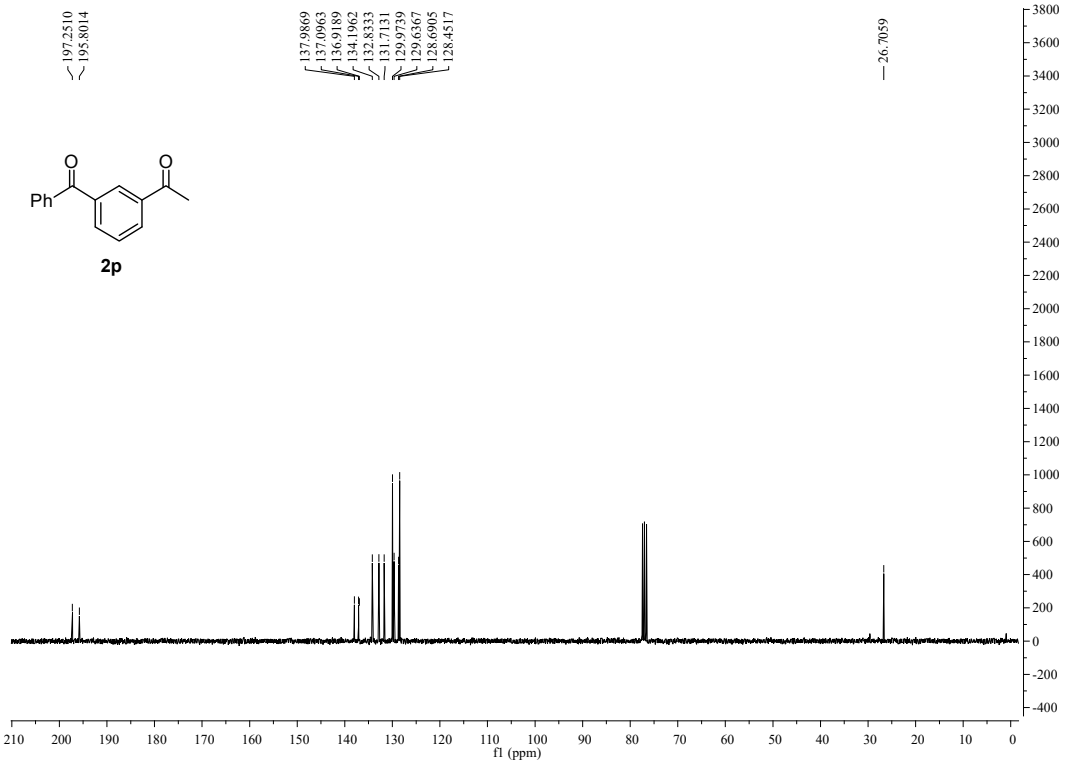
1.8028
1.6925
1.6789
4.00
3.99
2.10
f1 (ppm)
2o


212.0916
41.8667
26.9128
24.8781
f1 (ppm)
2o


8.3562
8.1620
7.9650
7.7788
7.6382
7.6164
7.5921
7.5671
7.5209
7.4963
7.4711
2.6408
Ph
O
O
2p
1.00
1.00
1.01
2.02
2.05
2.03
3.00
fl (ppm)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137.9869
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136.9189
134.1962
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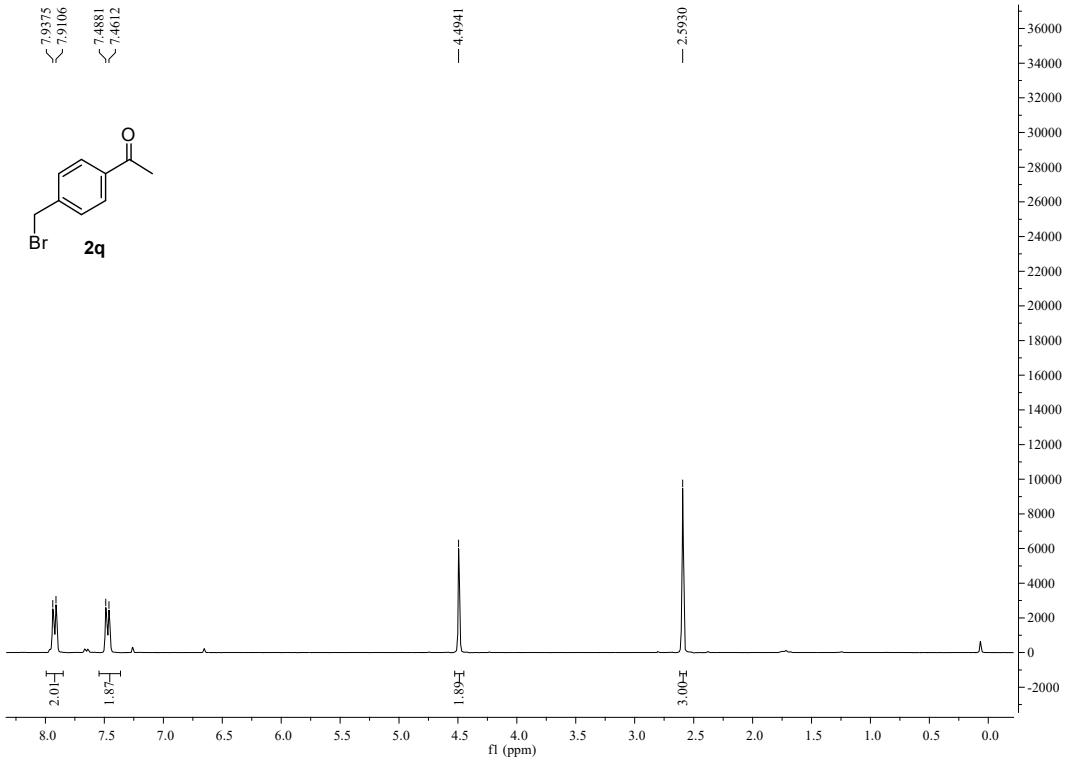
128.6905
128.4517
26.7059
Ph
O
O
2p
fl (ppm)


7.9375
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7.4881
7.4612
4.4941
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O
Br
2q
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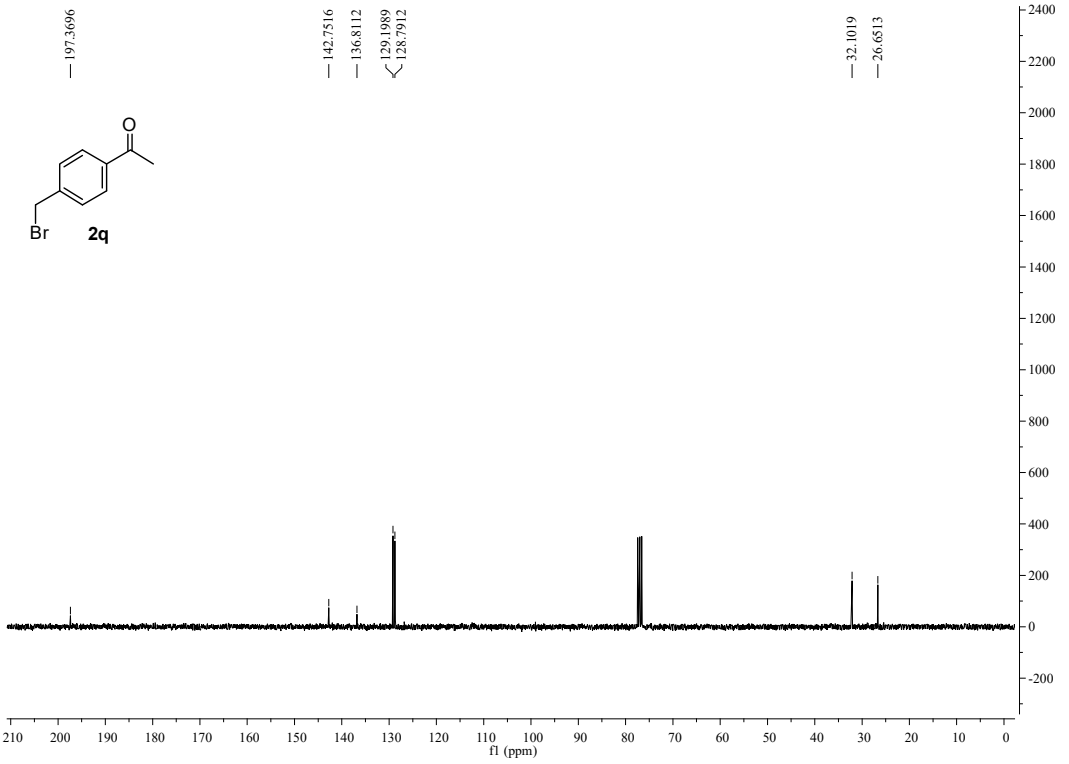
1.87
1.89
3.00
f1 (ppm)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142.7516
136.8112
129.1989
128.7912
32.1019
26.6513
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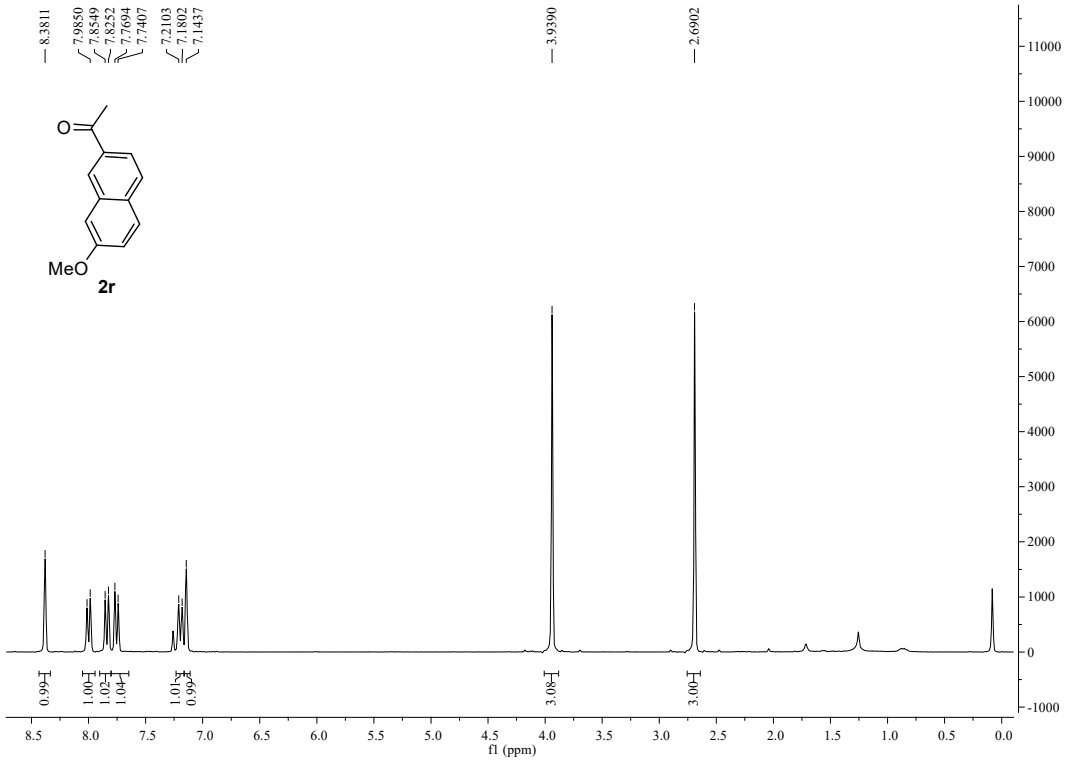
Br
2q
f1 (ppm)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7.9850
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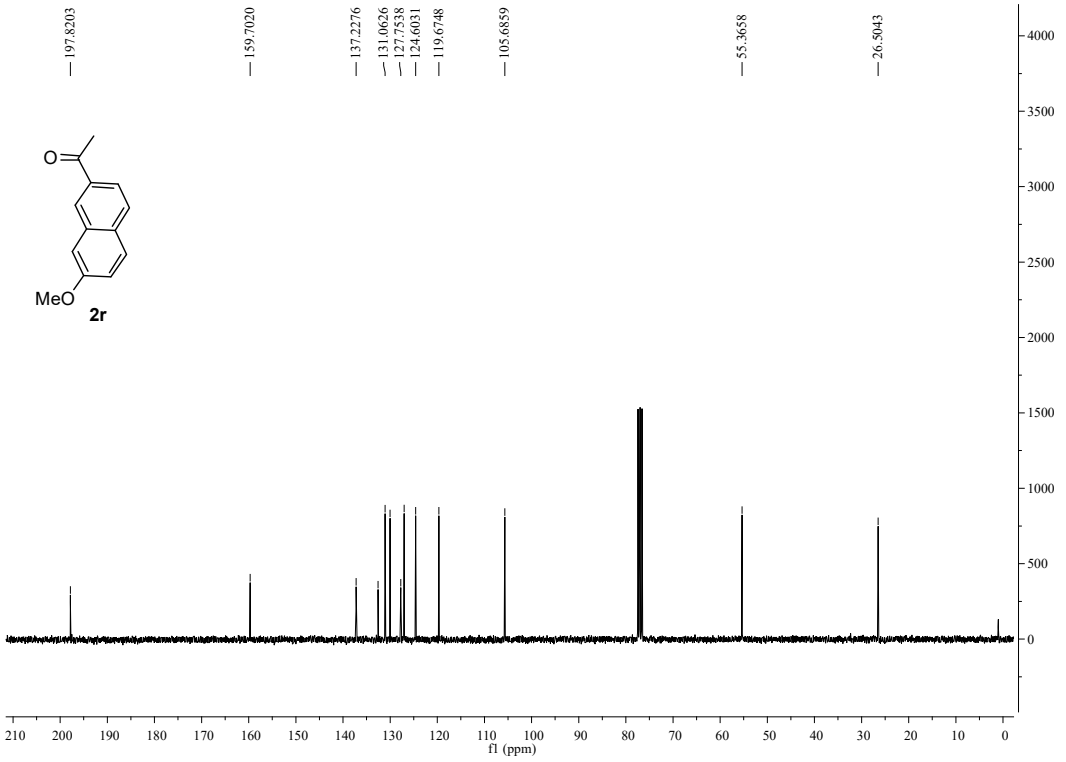
7.8252
7.7694
7.7407
7.2103
7.1802
7.1437
3.9390
2.6902
O
MeO
2r
0.99
1.00
1.02
1.04
1.01
0.99
3.08
3.00
f1 (ppm)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159.7020
137.2276
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124.6031
119.6748
105.6859
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26.5043
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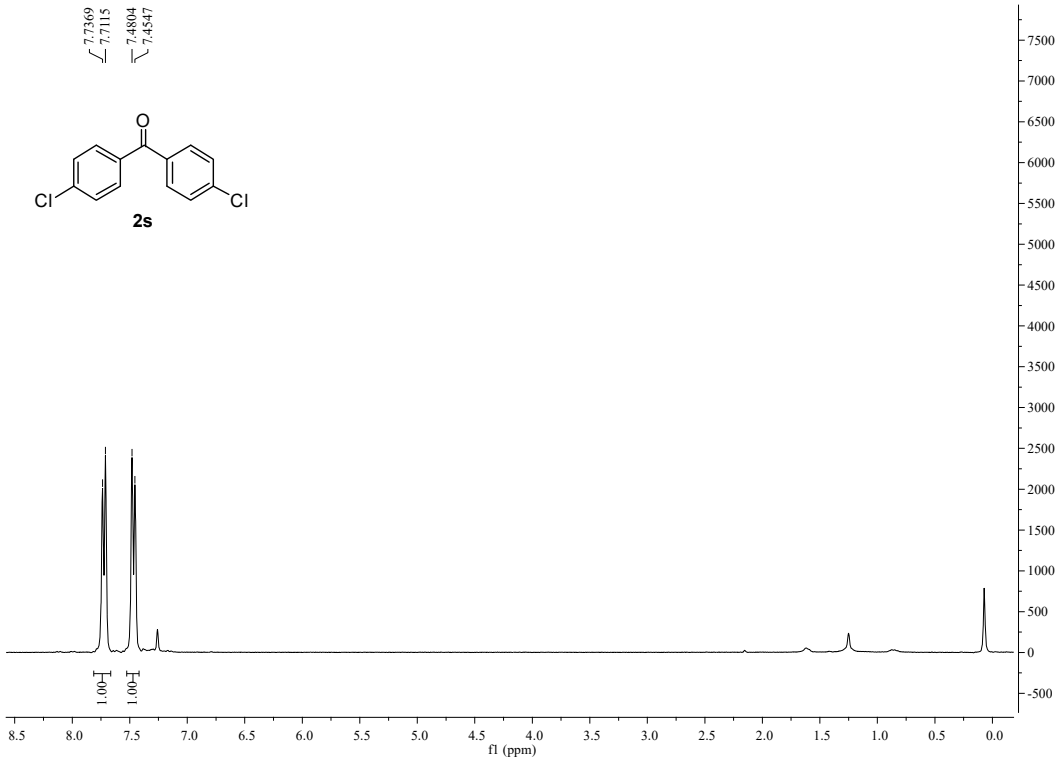
MeO
2r
f1 (ppm)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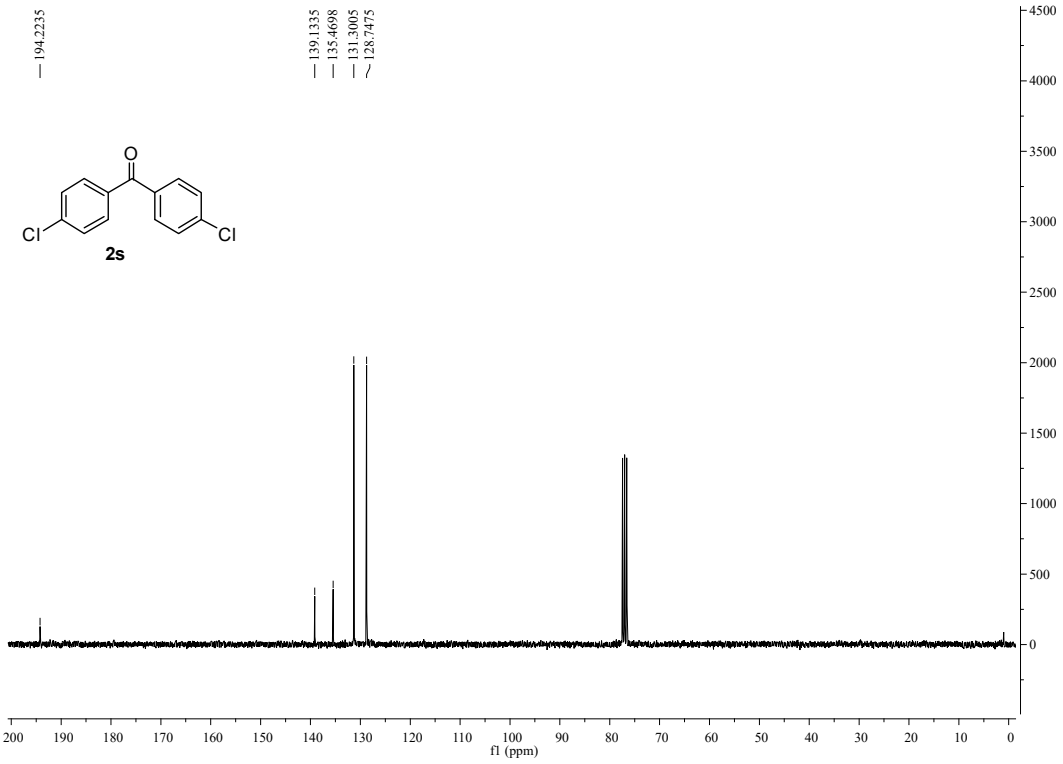
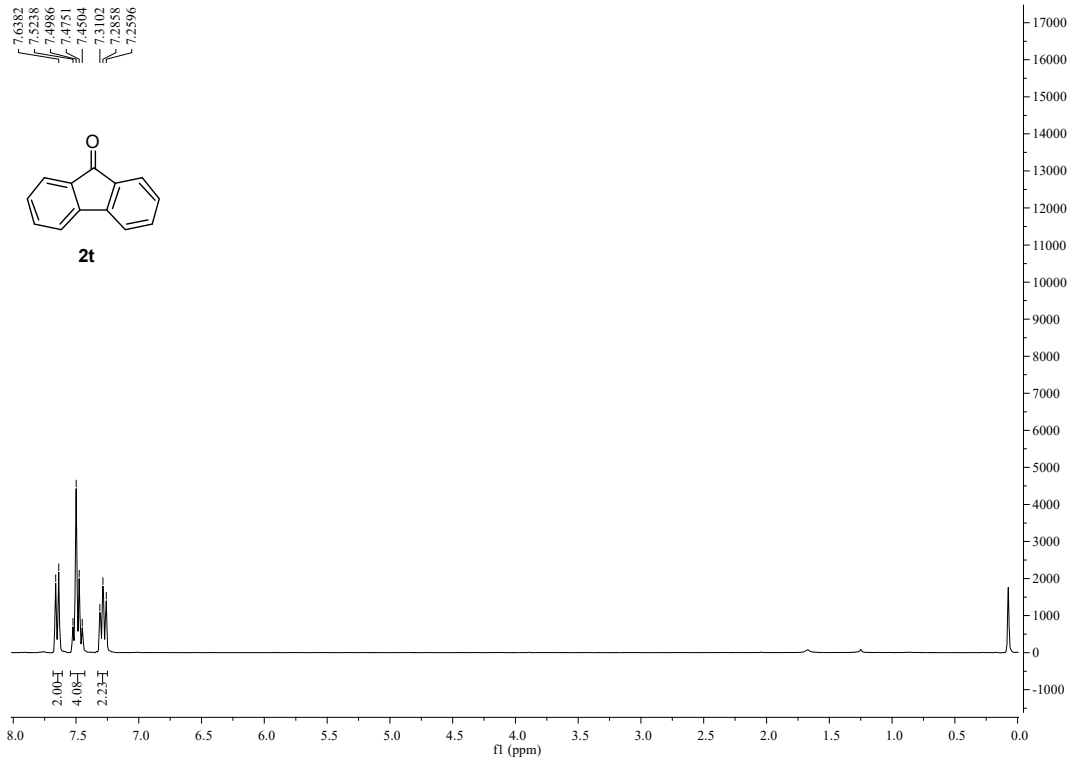
7.7115
7.4804
7.4547
O
Cl
Cl
2s
1.00
1.00
f1 (ppm)


194.2235
139.1335
135.4698
131.3005
128.7475
O
Cl
Cl
2s
f1 (ppm)


7.6382
7.5238
7.4986
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7.2596
O
2t
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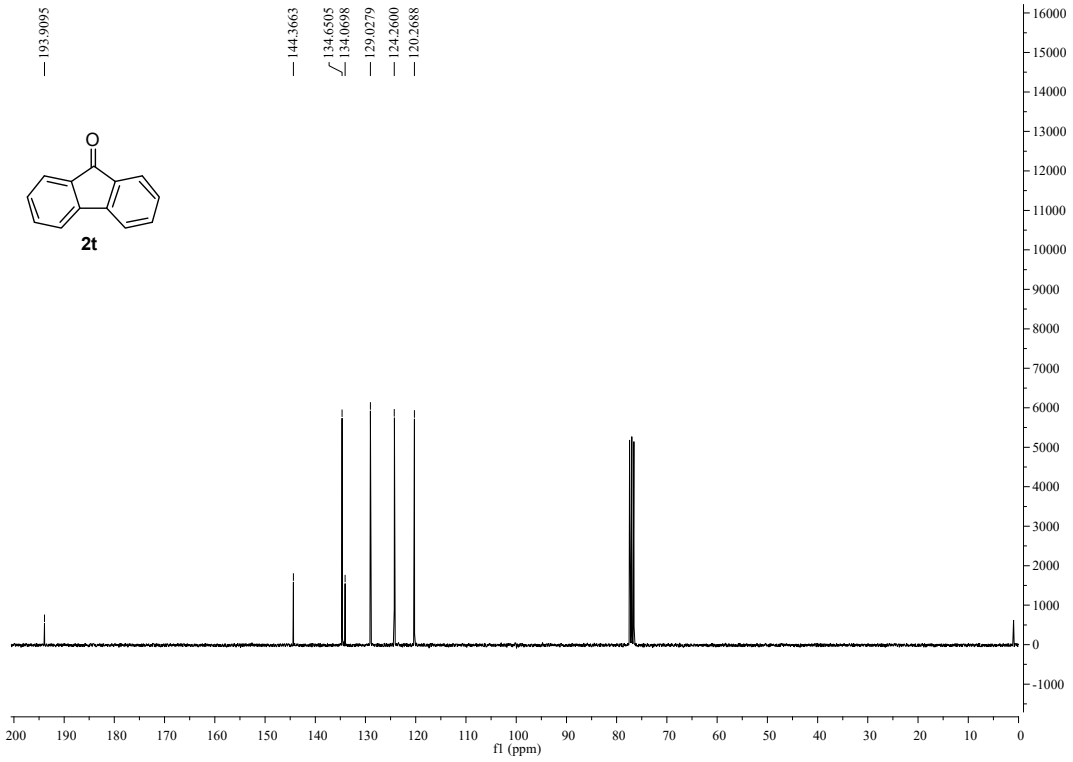
4.08
2.23
f1 (ppm)


193.9095
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129.0279
124.2600
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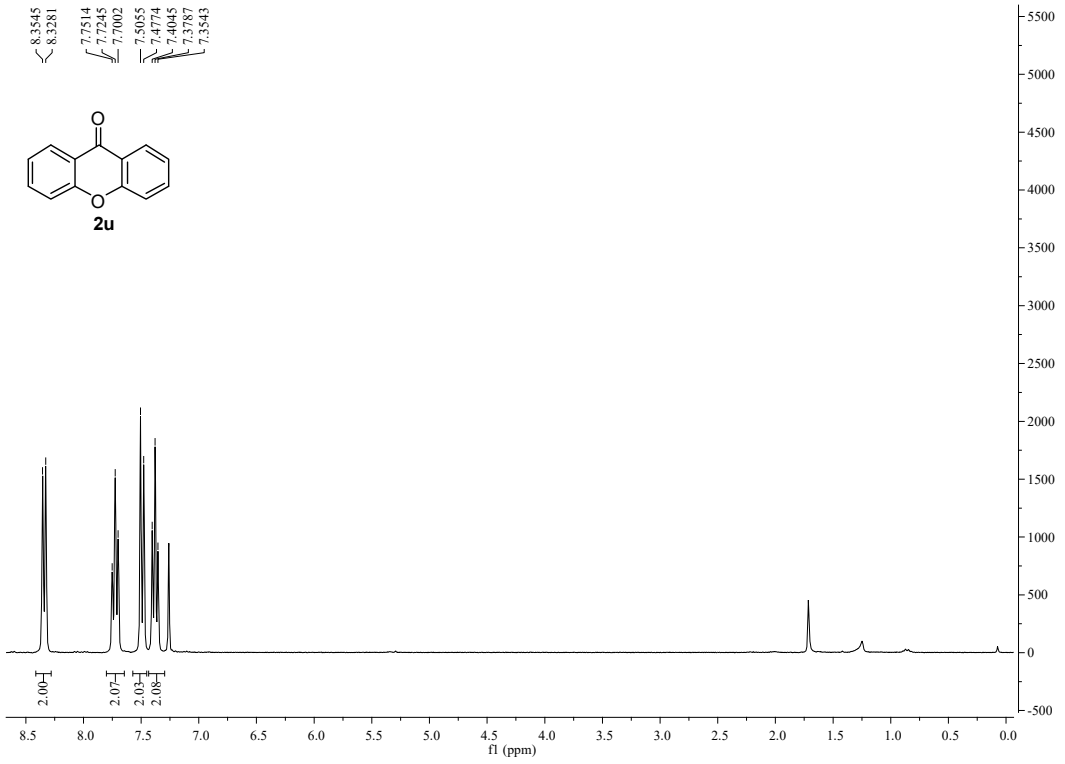
O
2t
f1 (ppm)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7.7514
7.7245
7.7002
7.5055
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O
O
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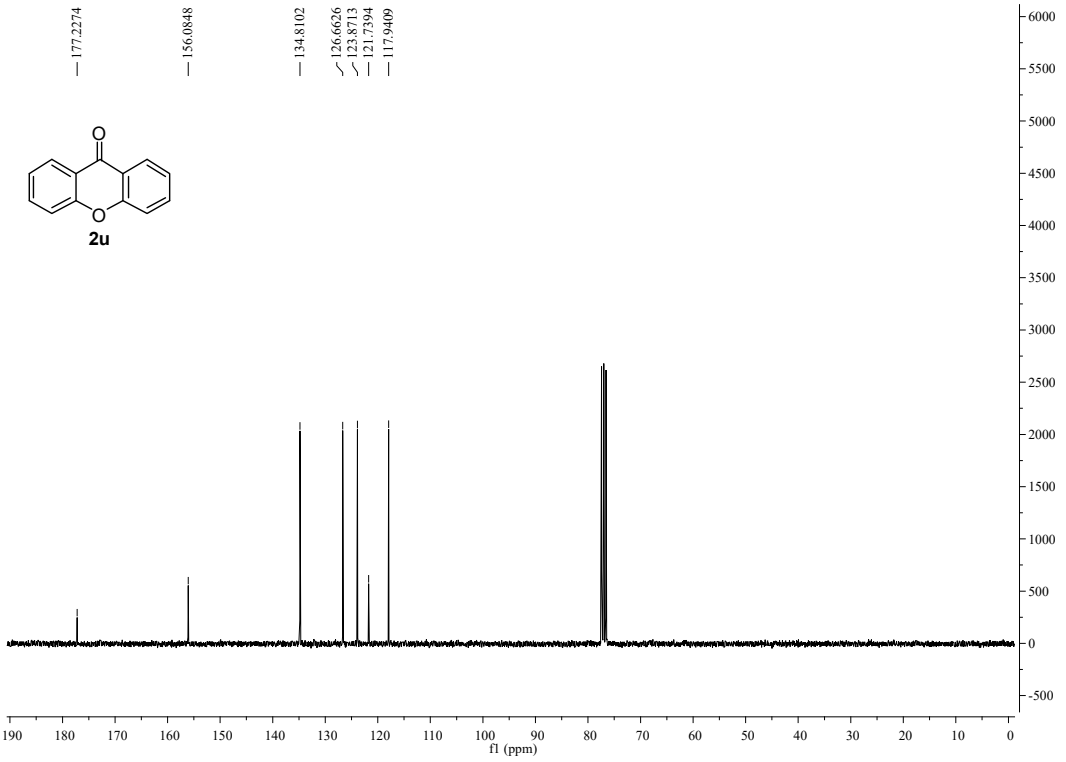
2.00
2.07
2.03
2.08
f1 (ppm)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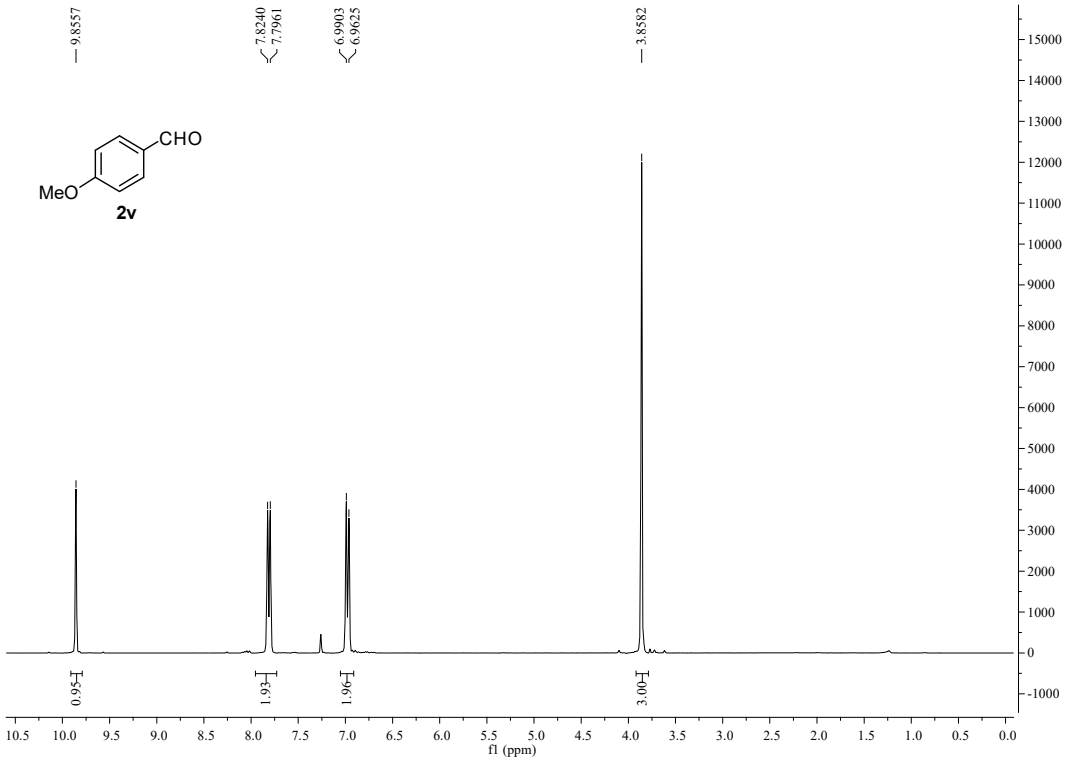
123.8713
121.7394
117.9409
O
O
2u
f1 (ppm)


9.8557
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6.9625
3.8582
CHO
MeO
2v
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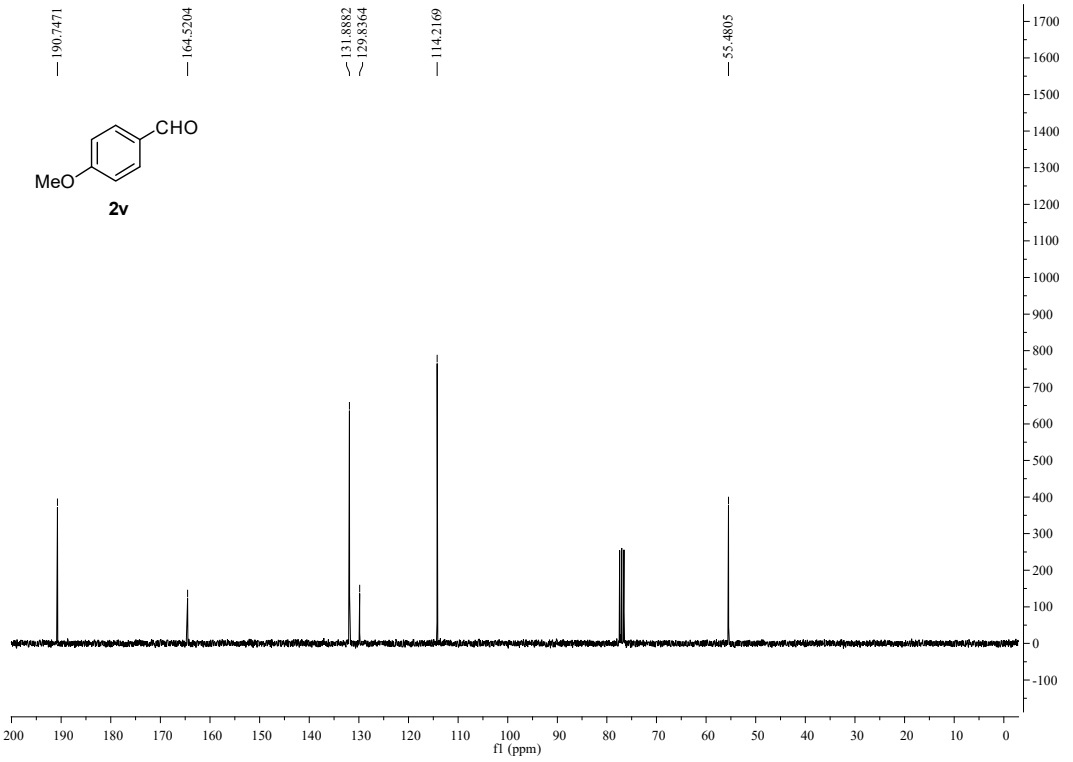
1.96
3.00
f1 (ppm)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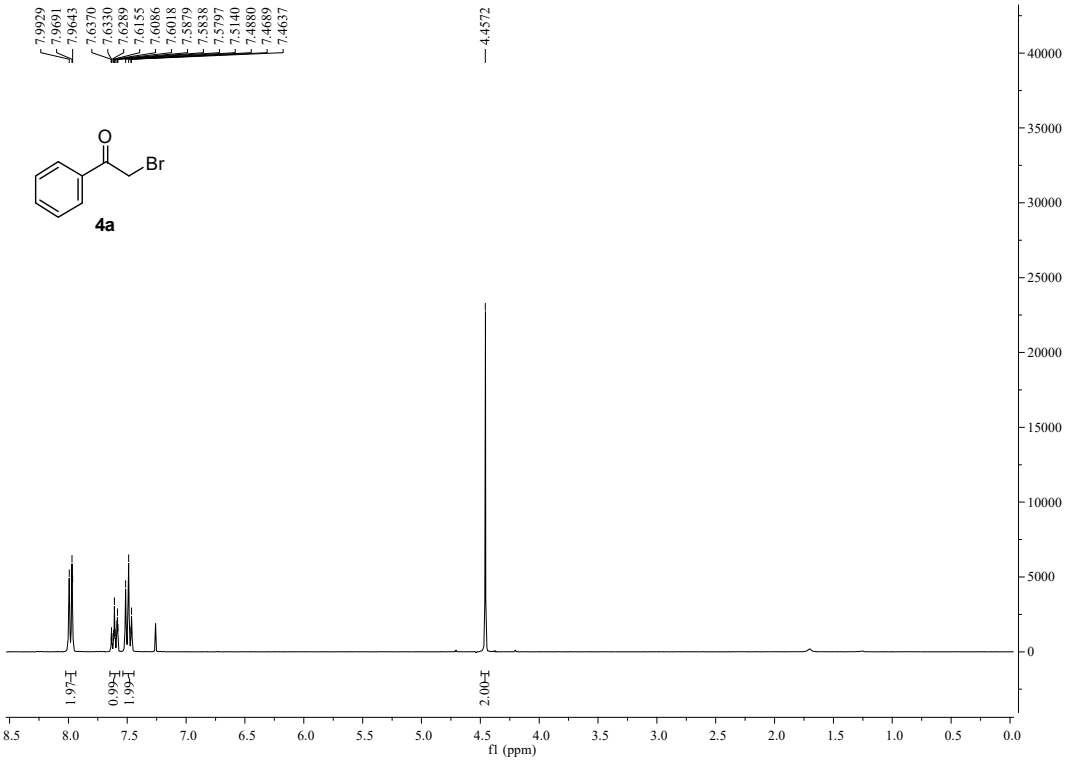
CHO
MeO
2v
f1 (ppm)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7.9643
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7.6330
7.6289
7.6155
7.6086
7.6018
7.5879
7.5838
7.5797
7.5140
7.4880
7.4689
7.4637
4.4572
O
Br
4a
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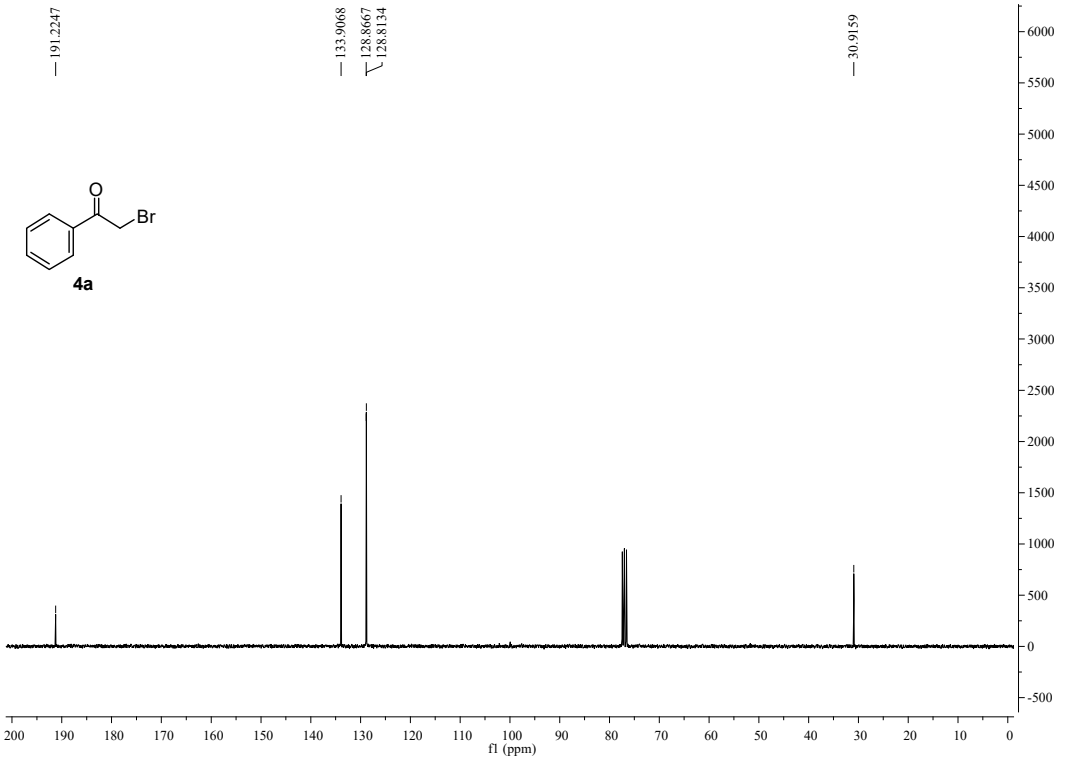
0.99
1.99
2.00
f1 (ppm)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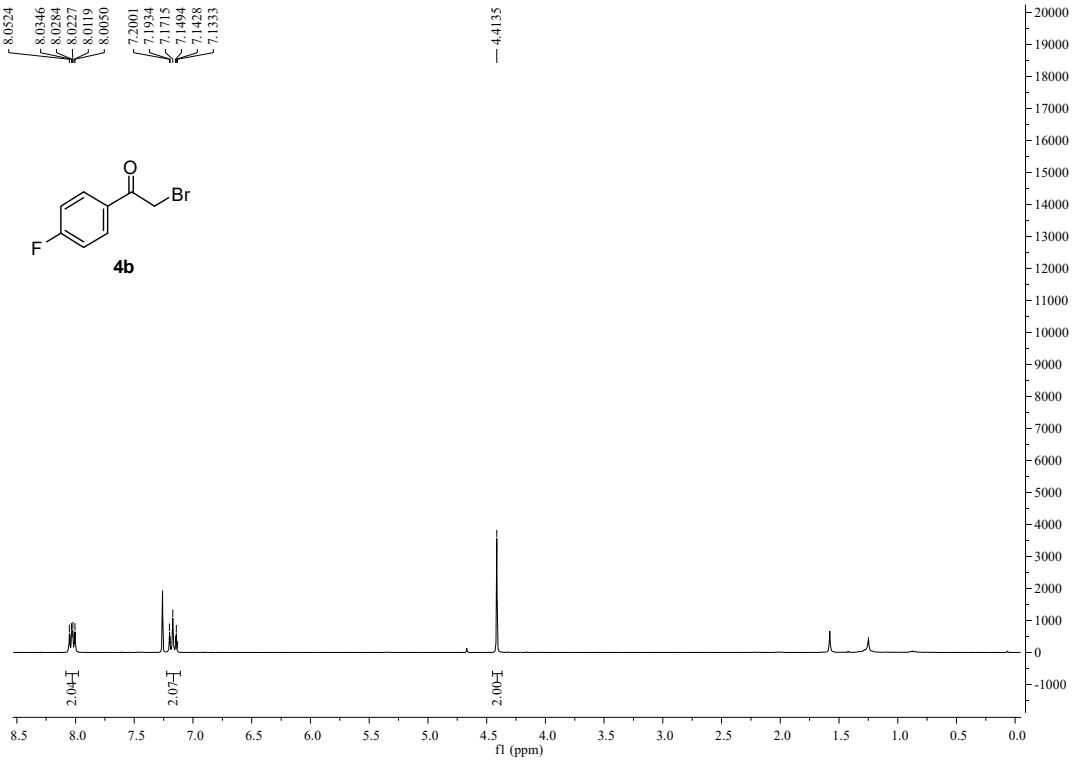
Br
4a
f1 (ppm)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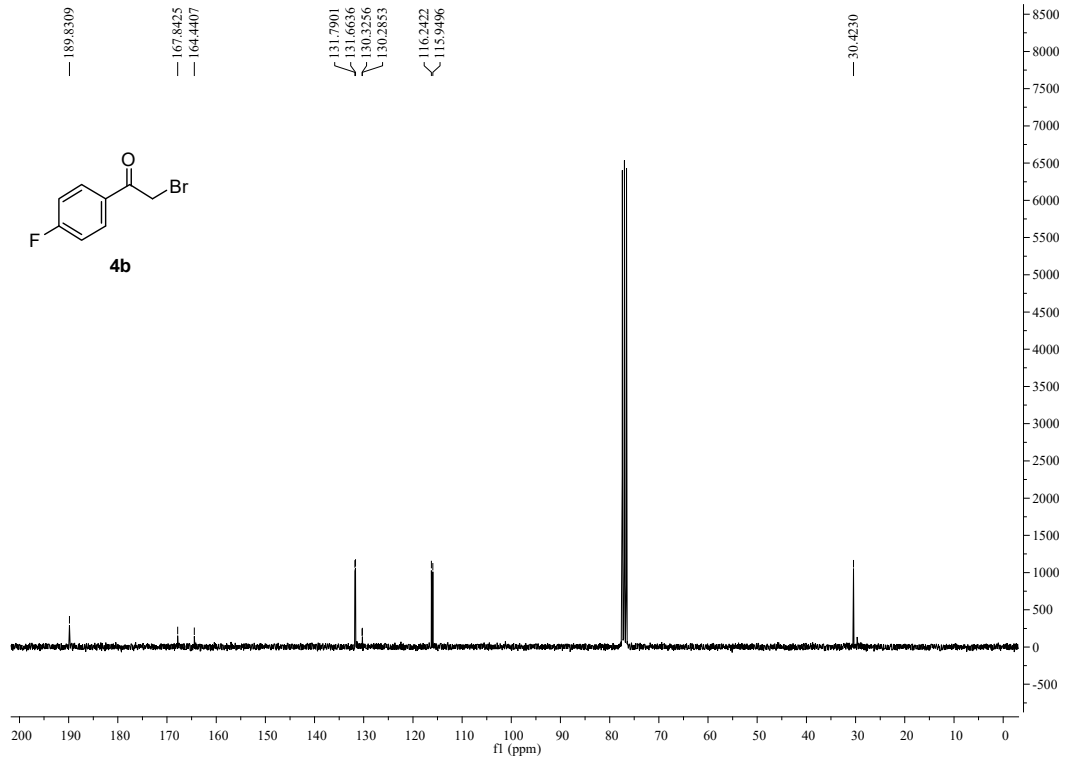
8.0284
8.0227
8.0119
8.0050
7.2001
7.1934
7.1715
7.1494
7.1428
7.1333
4.4135
O
Br
F
4b
2.04
2.07
2.00
f1 (ppm)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164.4407
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130.2853
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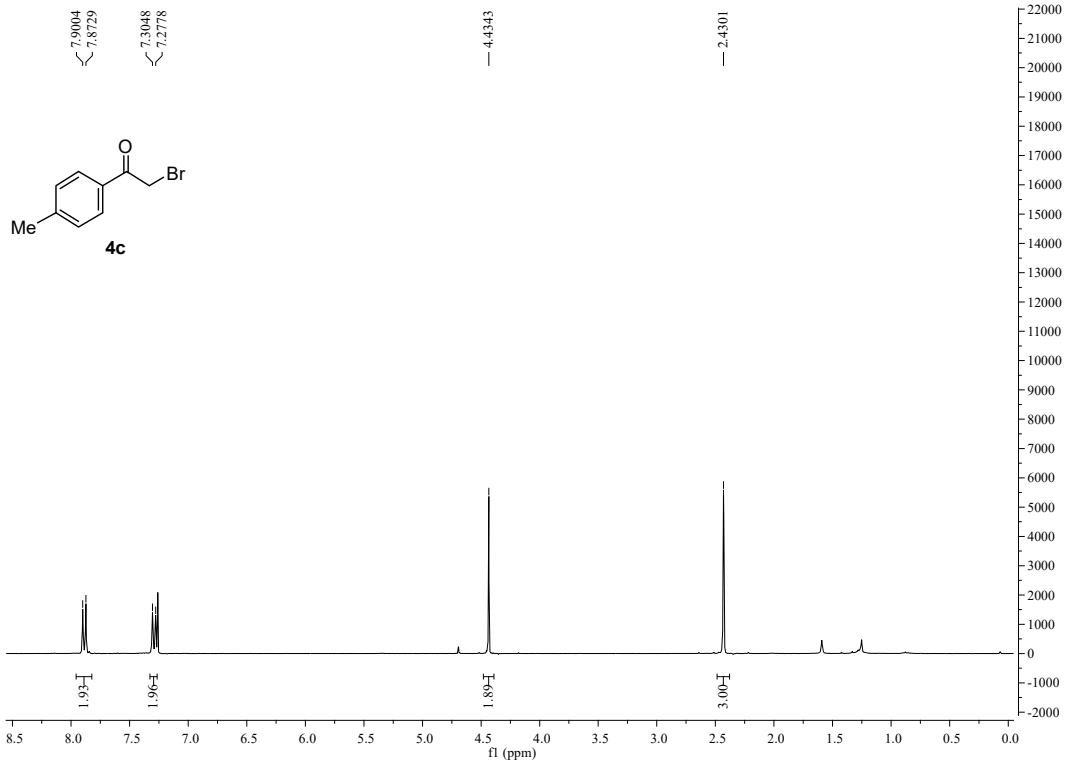
Br
F
4b
f1 (ppm)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2.4301
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Me
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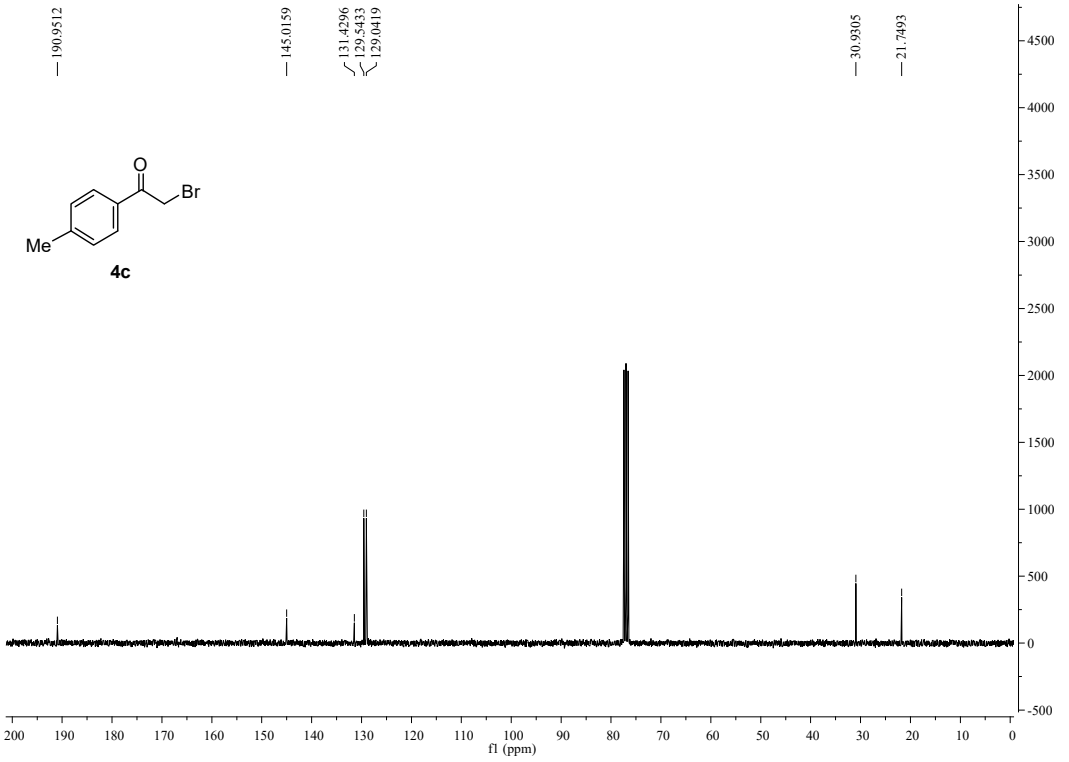
1.89
3.00
f1 (ppm)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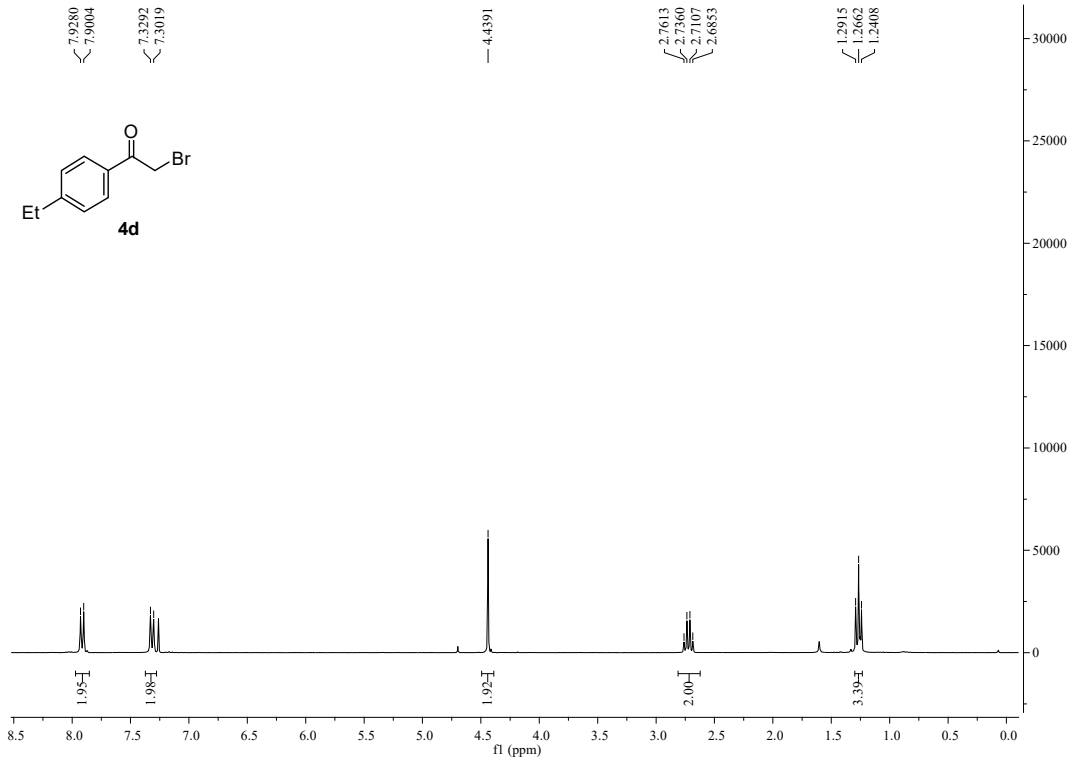
Br
Me
4c
f1 (ppm)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7.3019
4.4391
2.7613
2.7360
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2.6853
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O
Br
Et
4d
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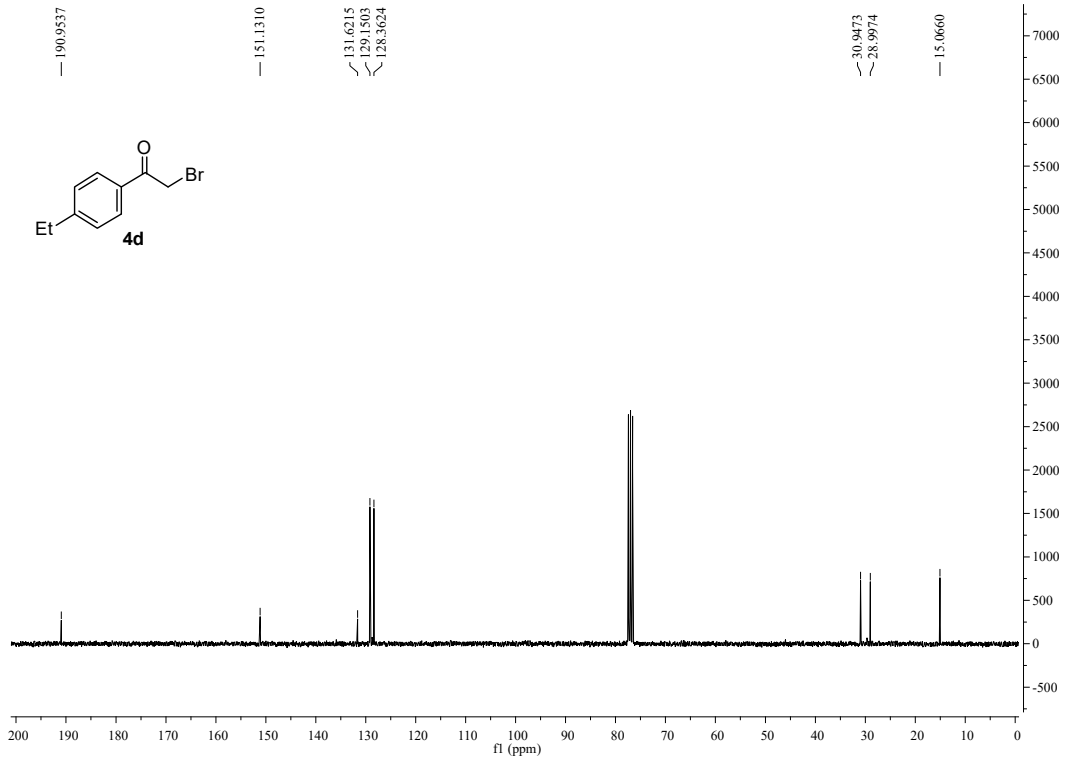
1.98
1.92
2.00
3.39
f1 (ppm)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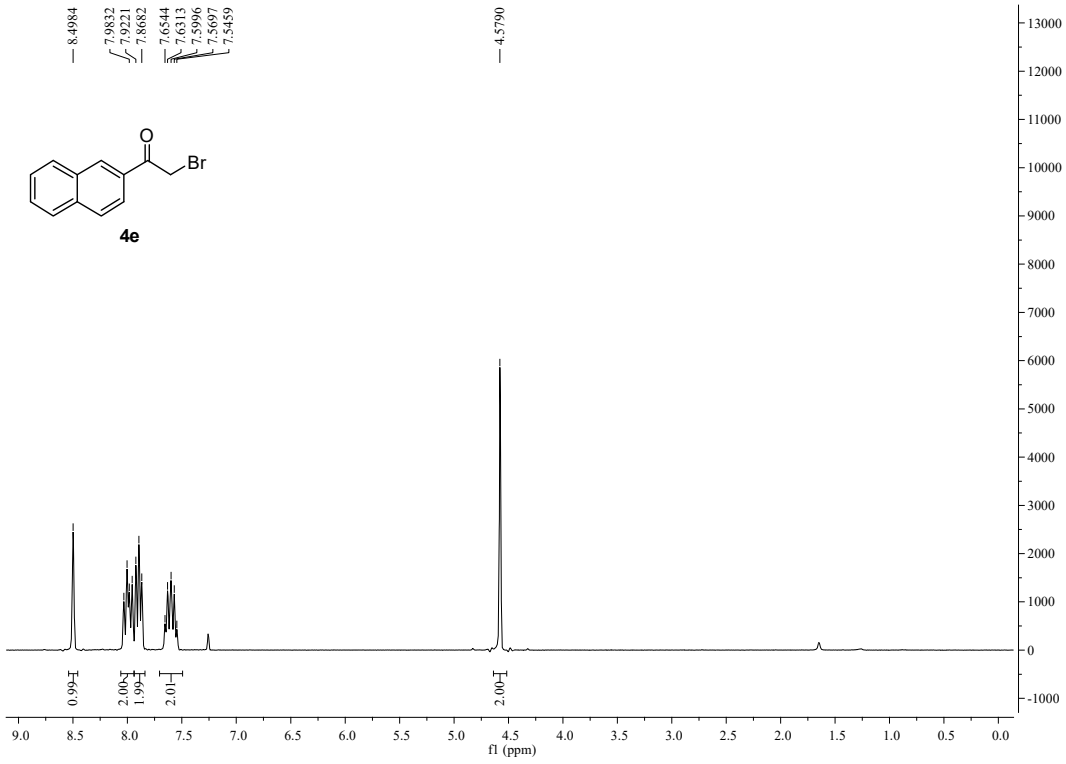
4d
f1 (ppm)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7.5996
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Br
4e
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1.99
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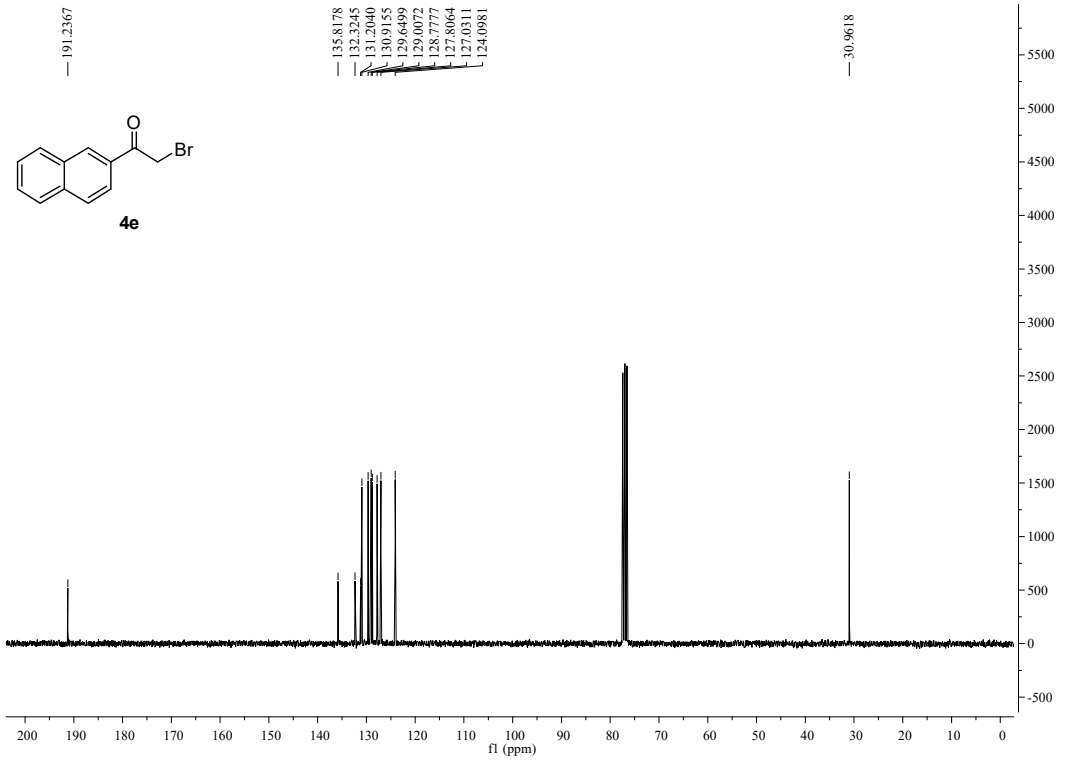
2.00
f1 (ppm)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30.9618
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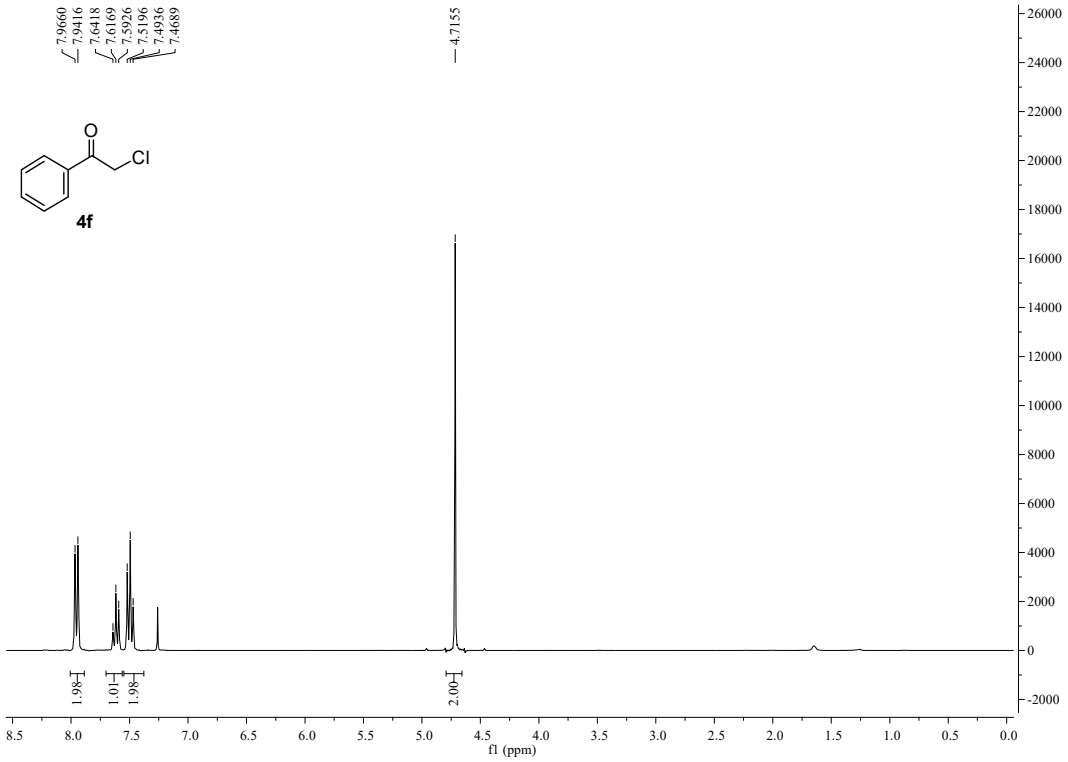
Br
4e
f1 (ppm)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7.4689
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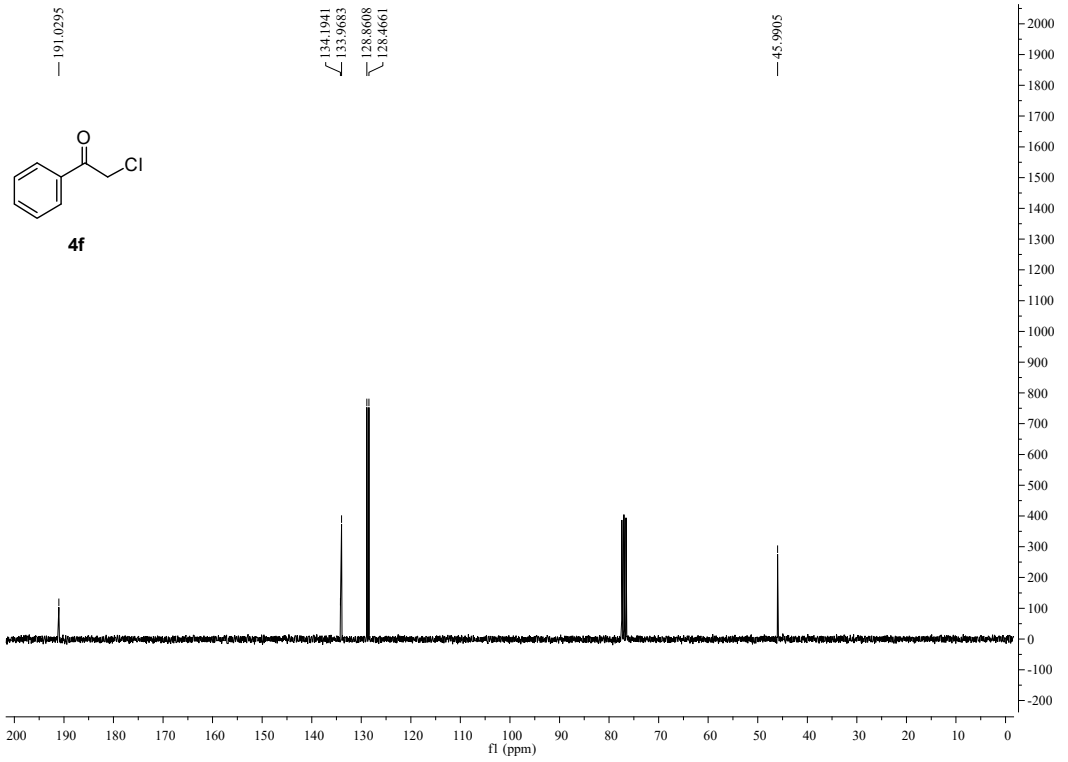
2.00
f1 (ppm)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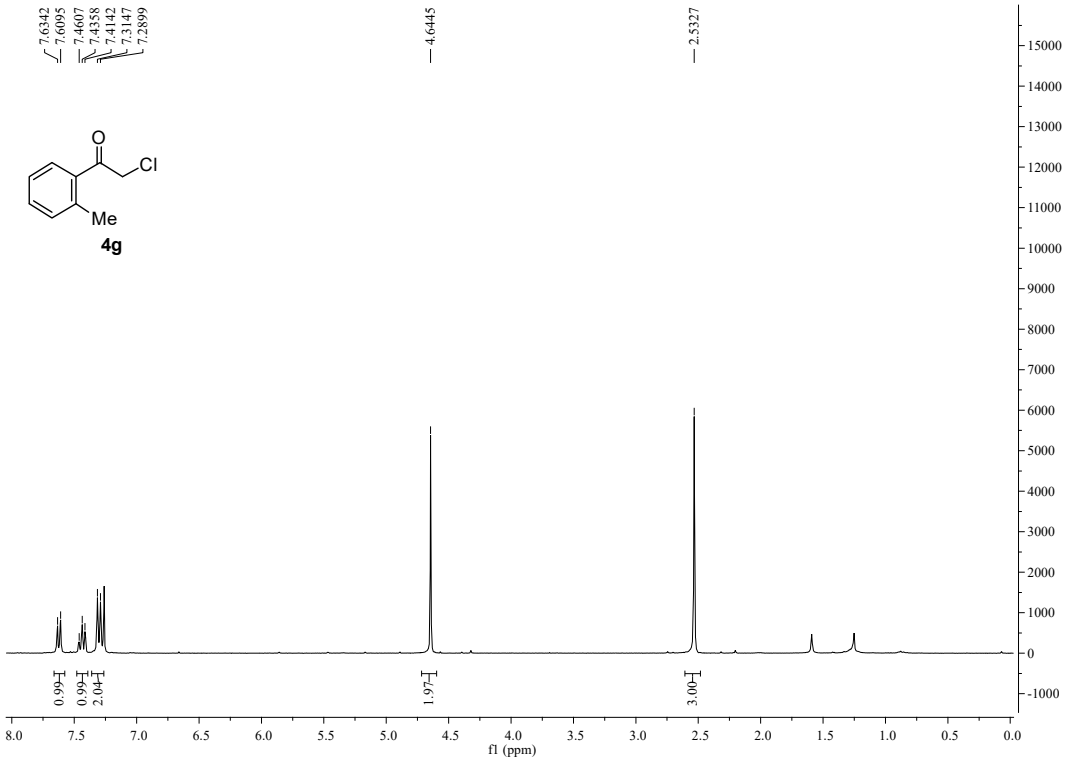
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Me
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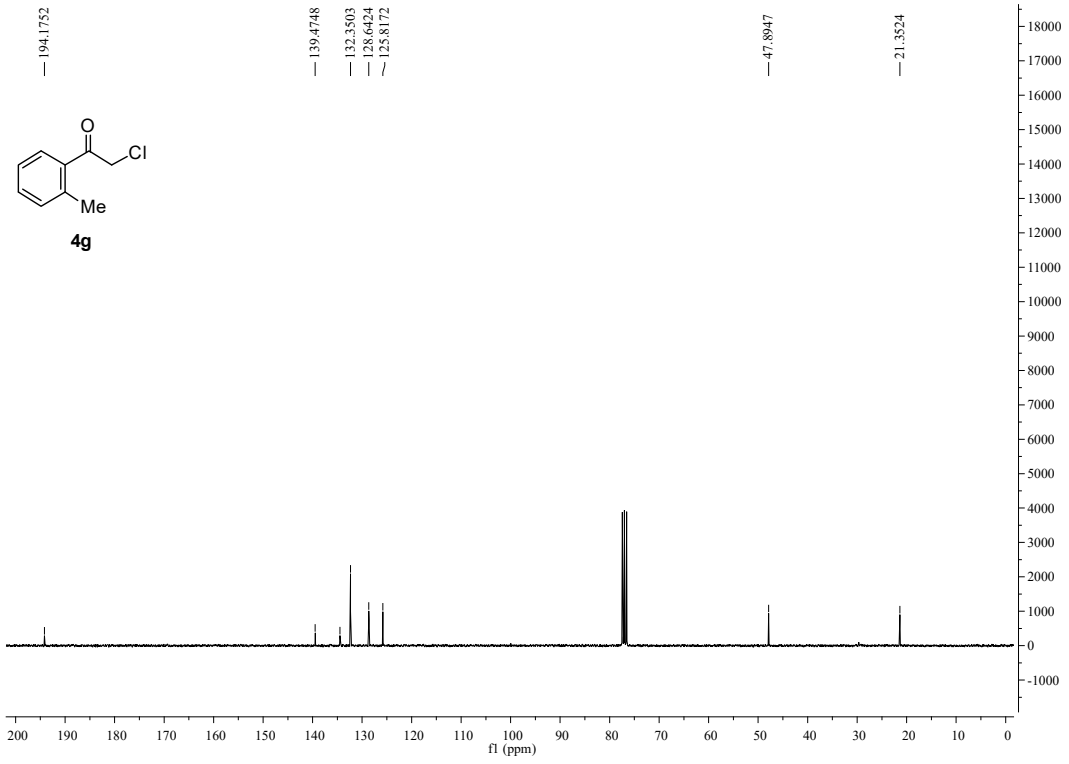
3.00
f1 (ppm)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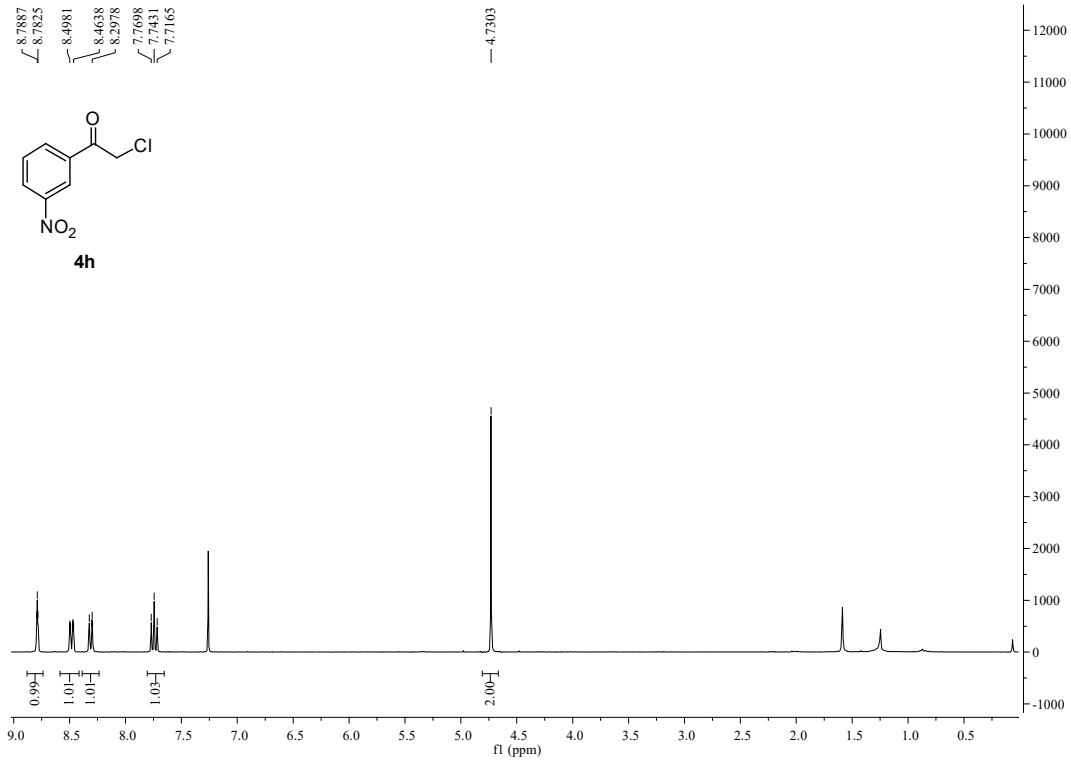
Me
4g
f1 (ppm)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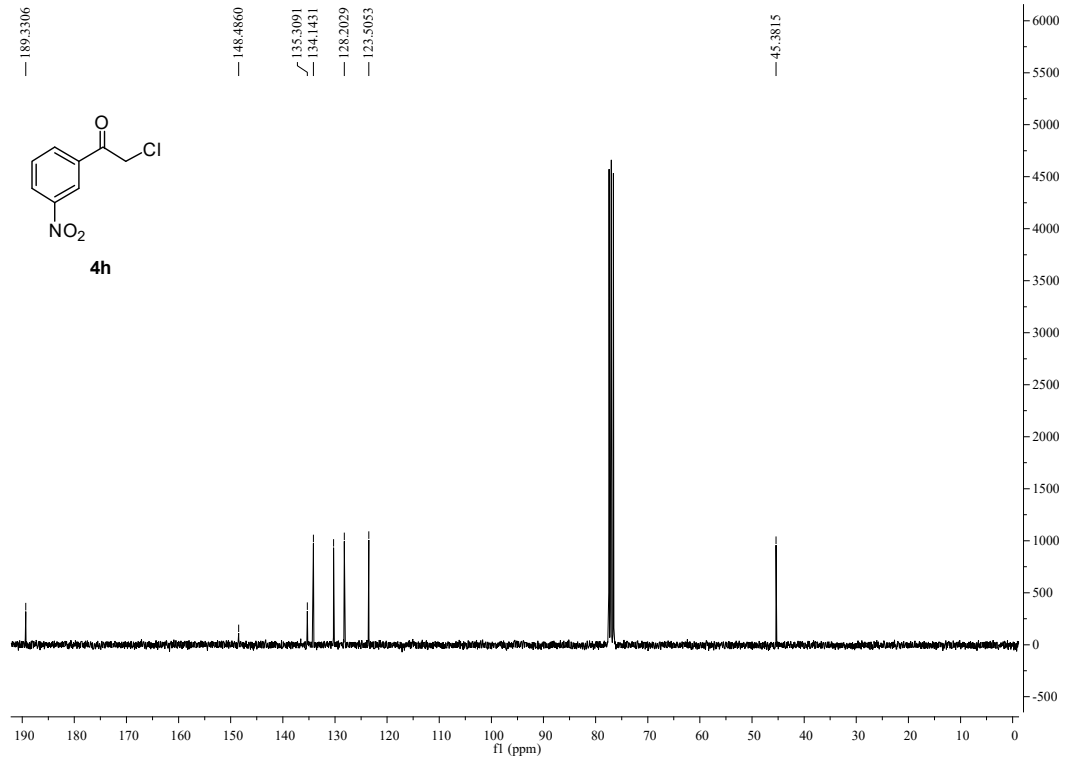
8.2978
7.7698
7.7431
7.7165
4.7303
O
Cl
NO2
4h
0.99
1.01
1.01
1.03
2.00
fl (ppm)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123.5053
45.3815
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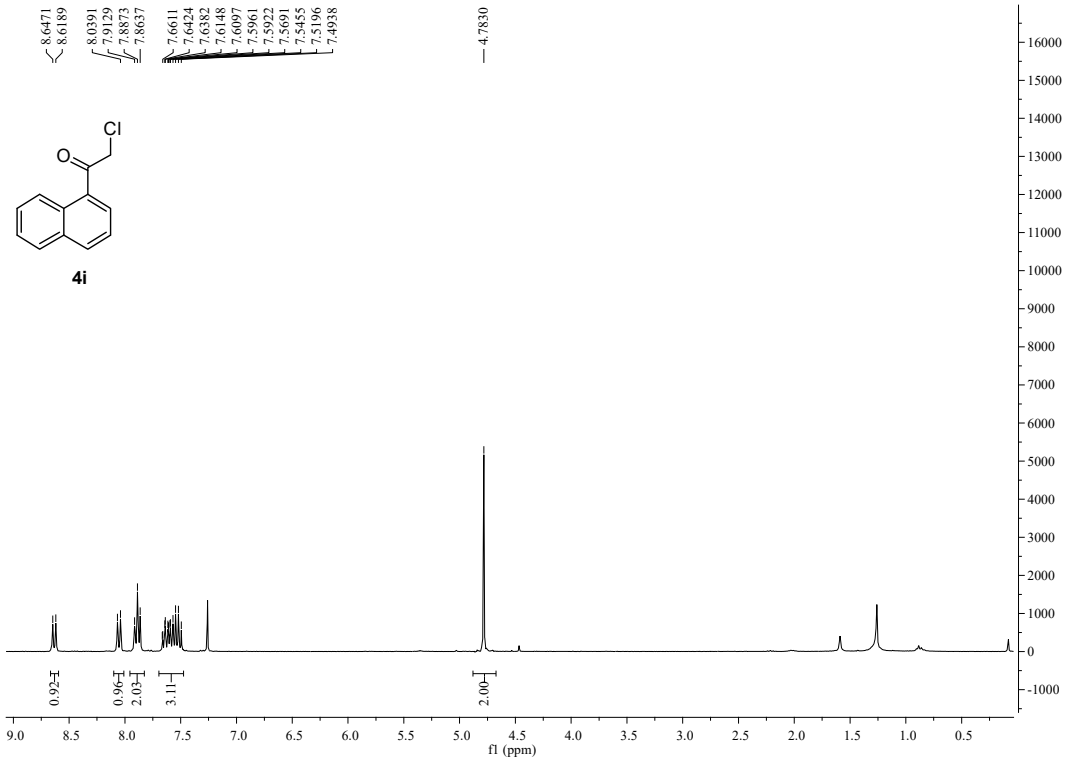
Cl
NO2
4h
fl (ppm)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8.0391
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7.6097
7.5961
7.5922
7.5691
7.5455
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4.7830
Cl
O
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0.96
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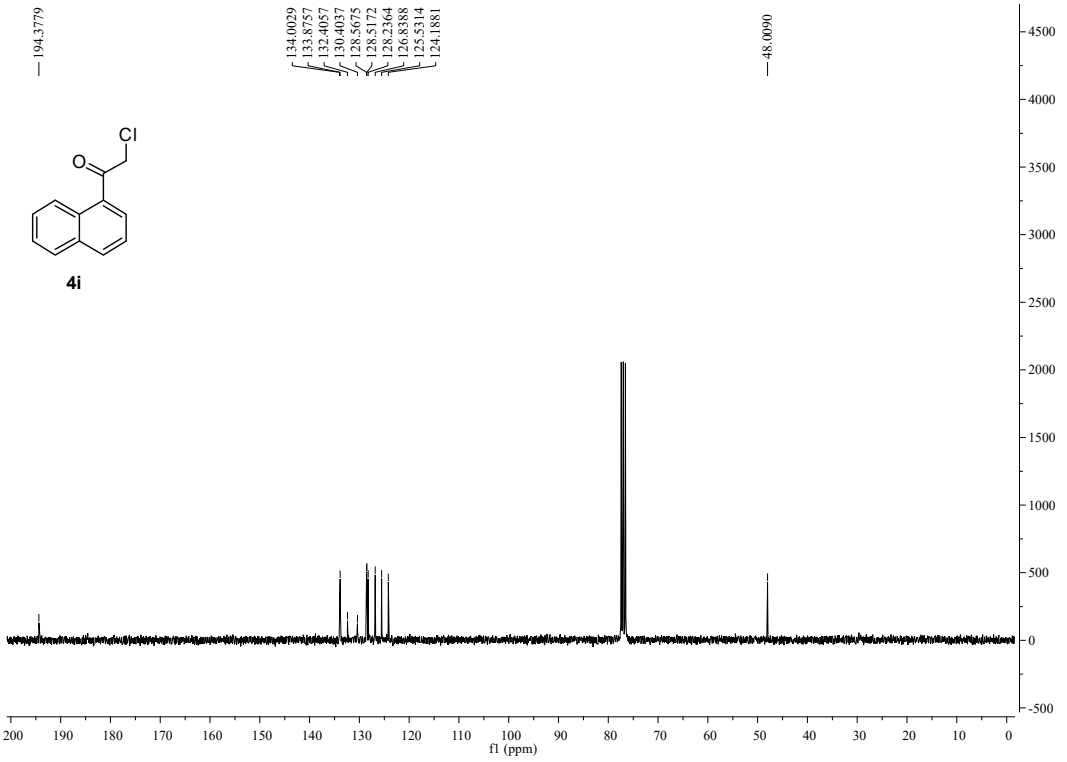
3.11
2.00
f1 (ppm)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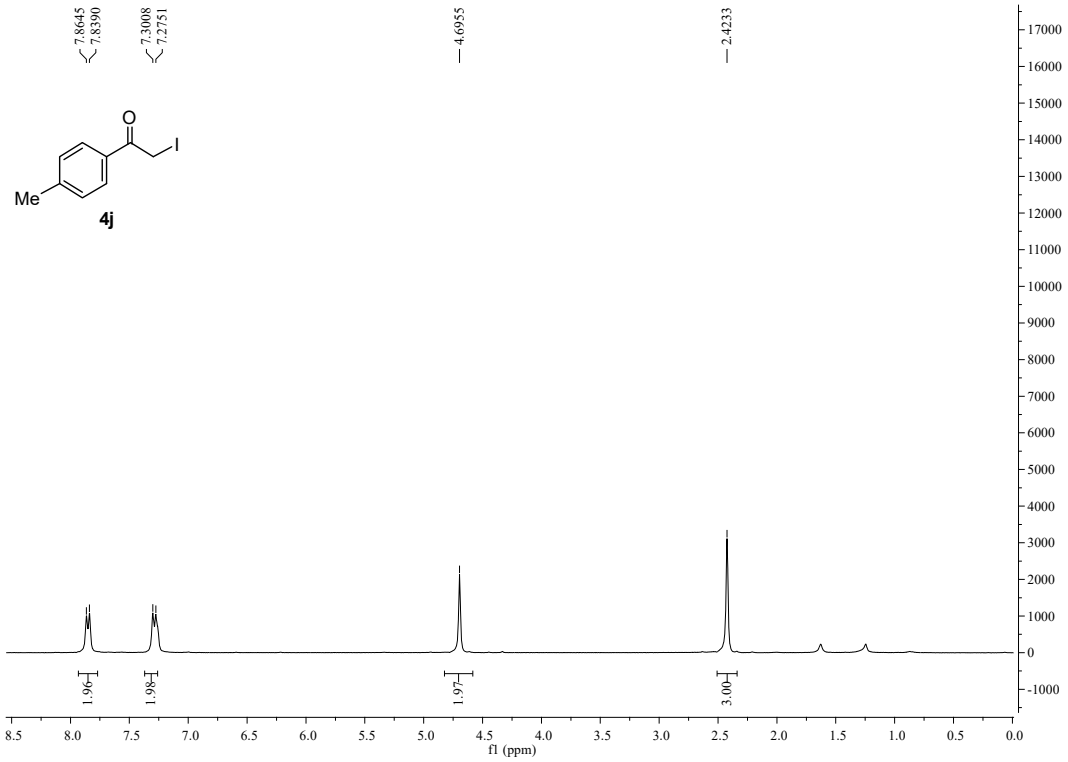
Cl
O
4i
f1 (ppm)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2.4233
O
I
Me
4j
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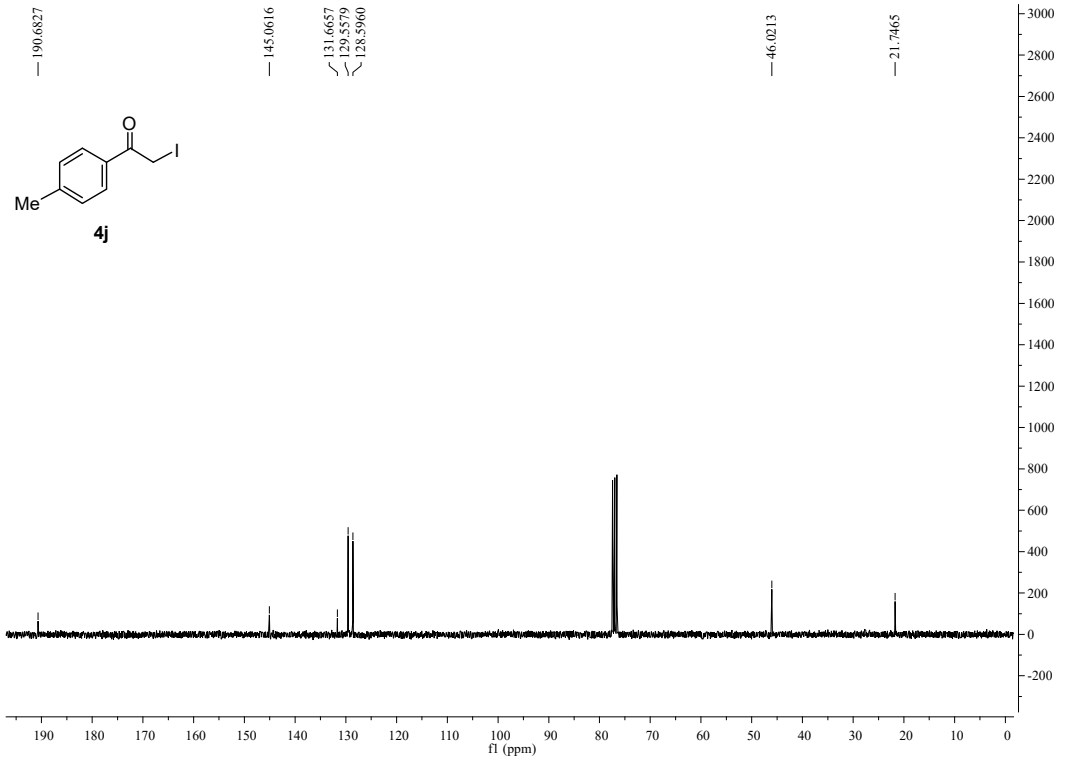
1.98
1.97
3.00
f1 (ppm)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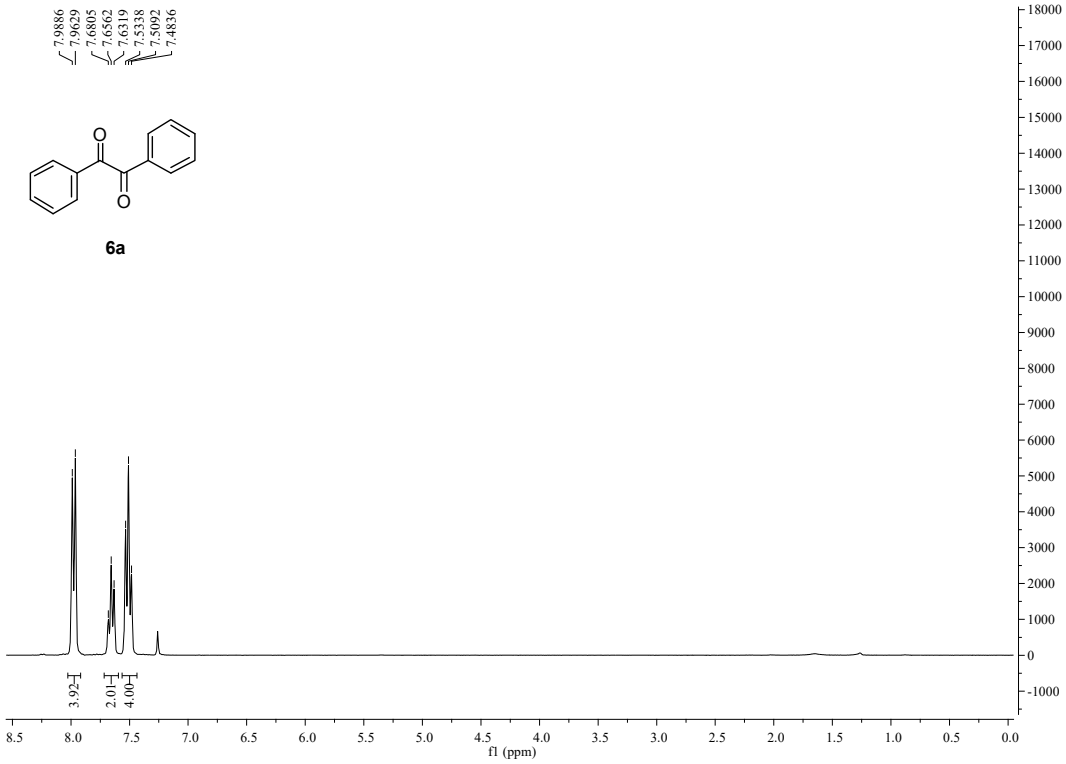
131.6657
129.5579
128.5960
46.0213
21.7465
O
I
Me
4j
f1 (ppm)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7.6805
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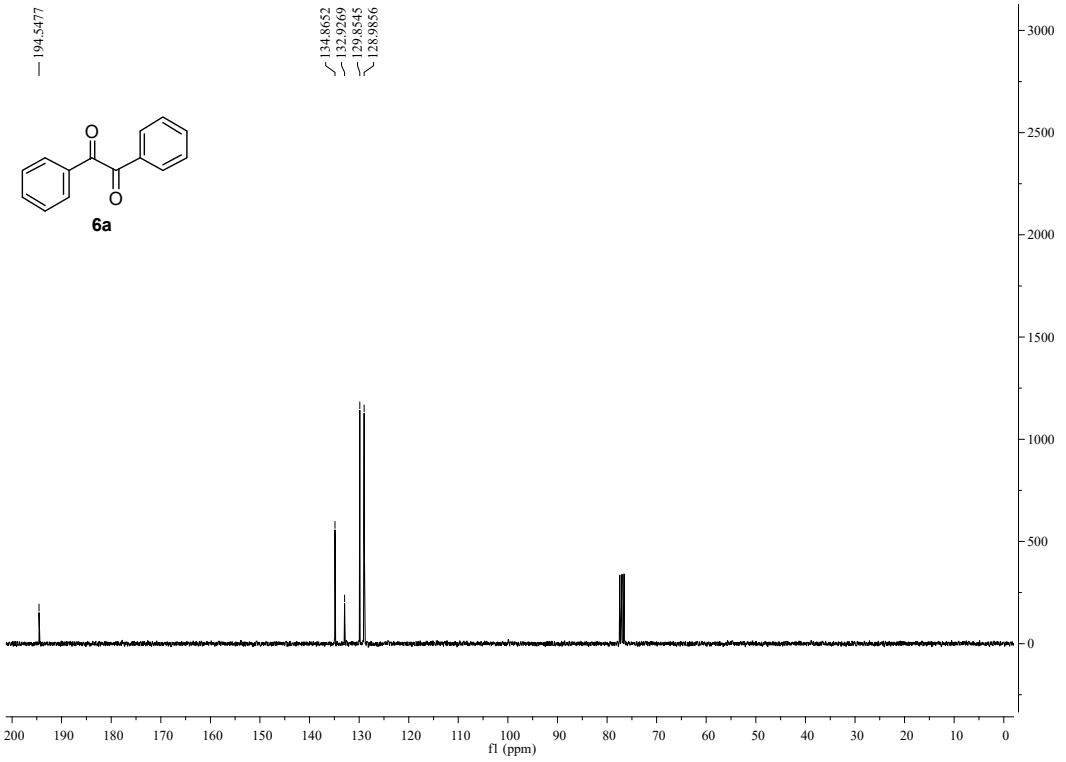
7.5338
7.5092
7.4836
O
O
6a
3.92
2.01
4.00
f1 (ppm)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132.9269
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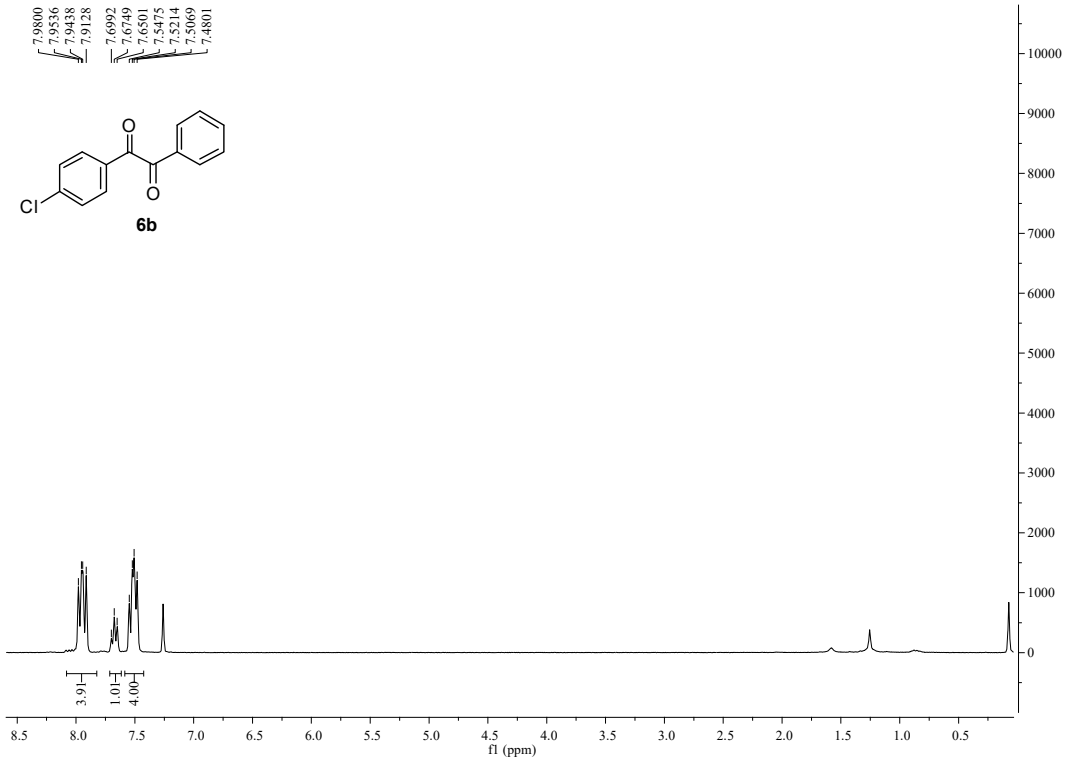
128.9856
O
O
6a
f1 (ppm)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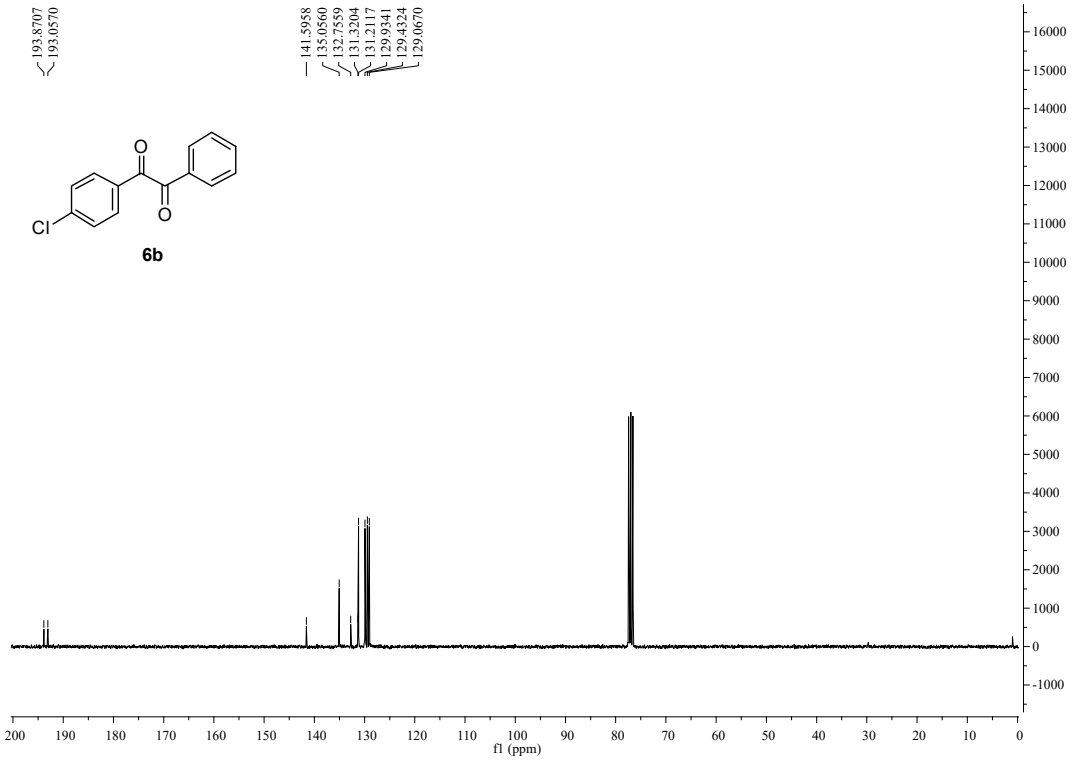
7.9438
7.9128
7.6992
7.6749
7.6501
7.5475
7.5214
7.5069
7.4801
O
O
Cl
6b
3.91
1.01
4.00
f1 (ppm)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193.0570
141.5958
135.0560
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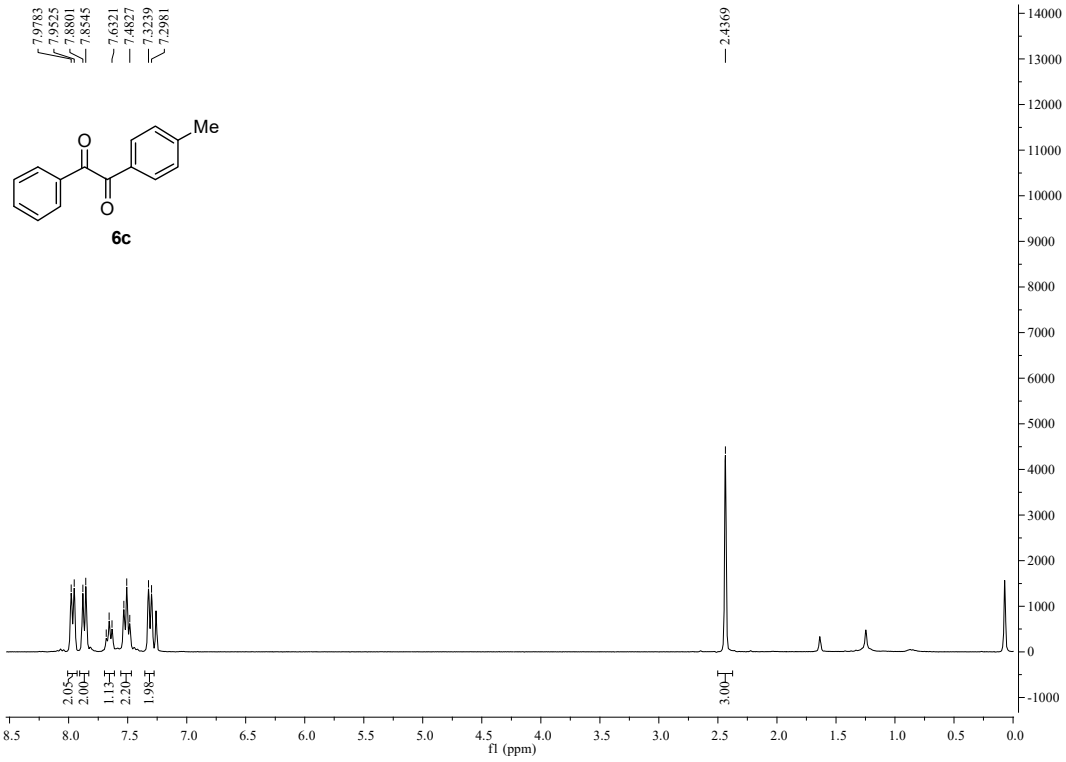
131.3204
131.2117
129.9341
129.4324
129.0670
O
O
Cl
6b
f1 (ppm)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7.9525
7.8801
7.8545
7.6321
7.4827
7.3239
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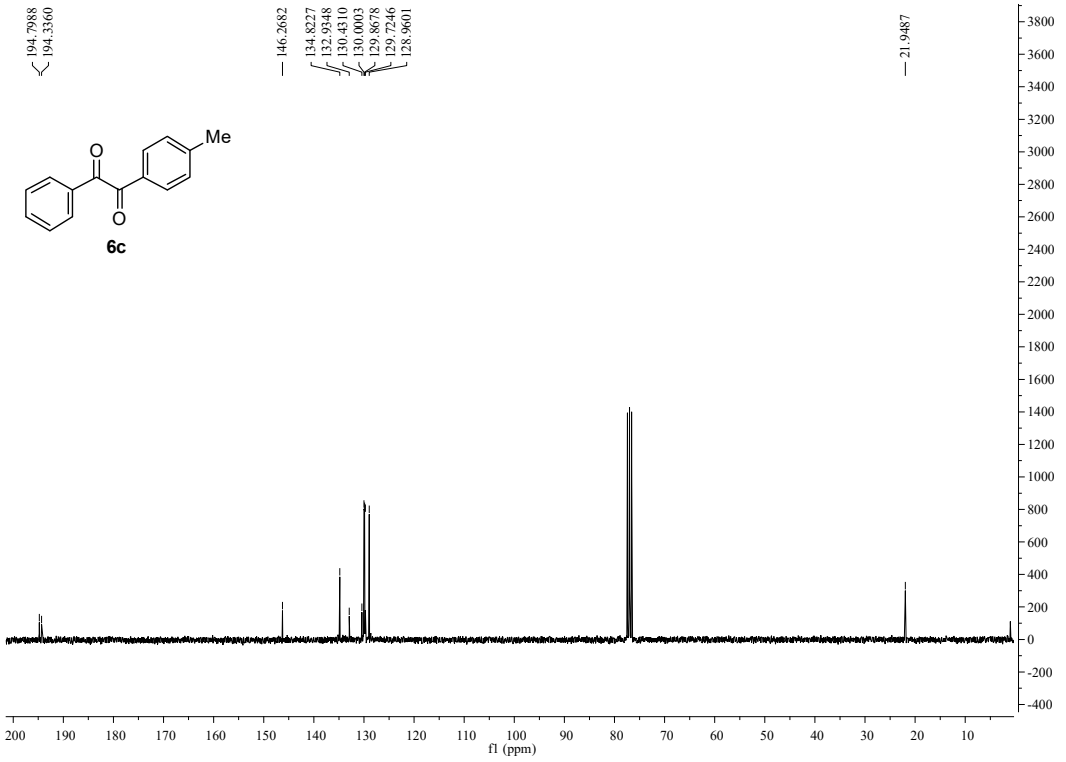
2.4369
Me
O
O
6c
2.05
2.00
1.13
2.20
1.98
3.00
fl (ppm)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146.2682
134.8227
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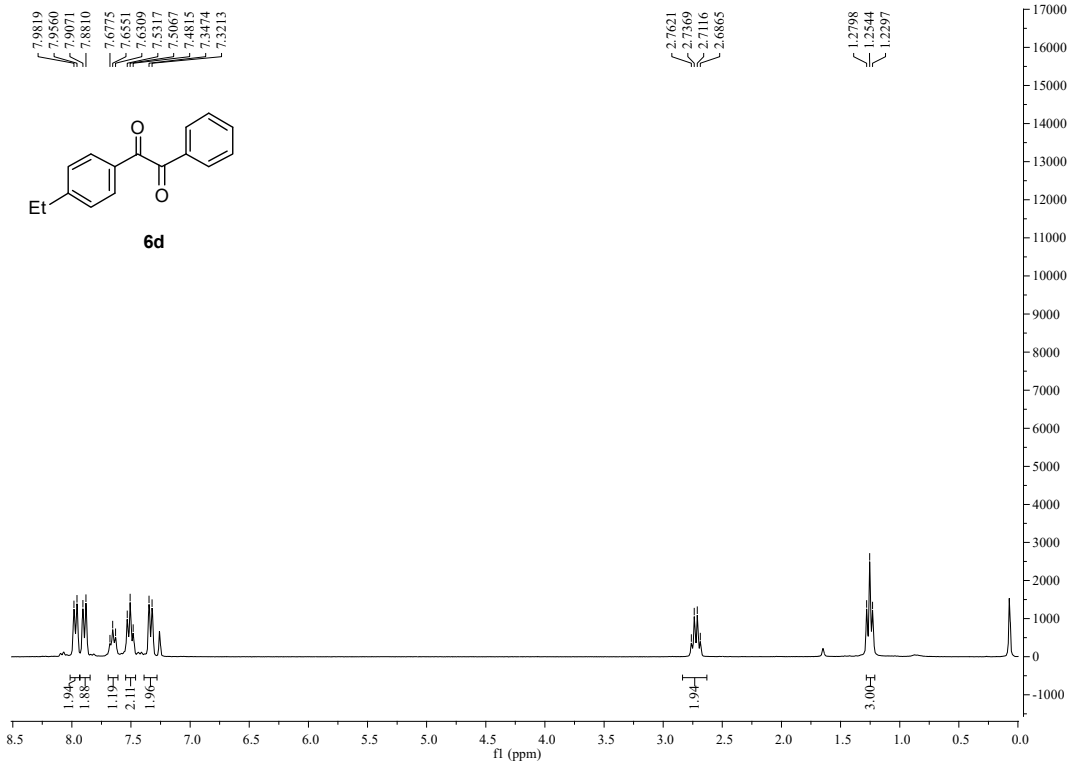
130.4310
130.0003
129.8678
129.7246
128.9601
21.9487
Me
O
O
6c
fl (ppm)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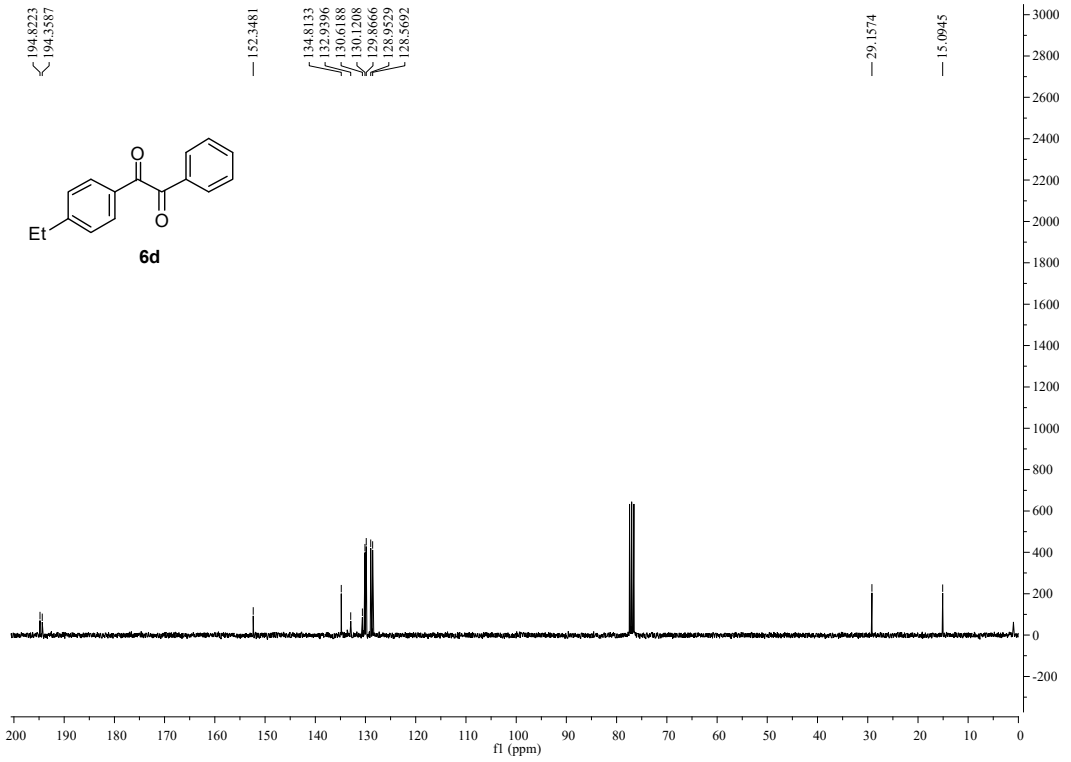
7.9071
7.8810
7.6775
7.6551
7.6309
7.5317
7.5067
7.4815
7.3474
7.3213
2.7621
2.7369
2.7116
2.6865
1.2798
1.2544
1.2297
O
O
Et
6d
1.94
1.88
1.19
2.11
1.96
1.94
3.00
f1 (ppm)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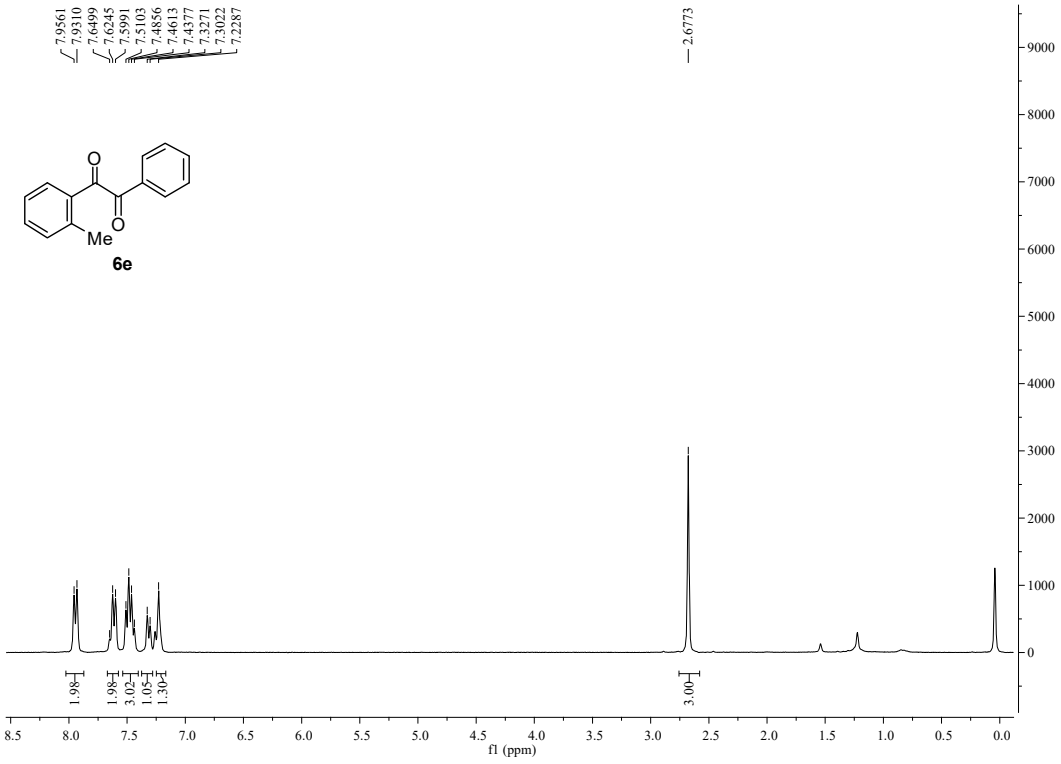
152.3481
134.8133
132.9396
130.6188
130.1208
129.8666
128.9529
128.5692
29.1574
15.0945
O
O
Et
6d
f1 (ppm)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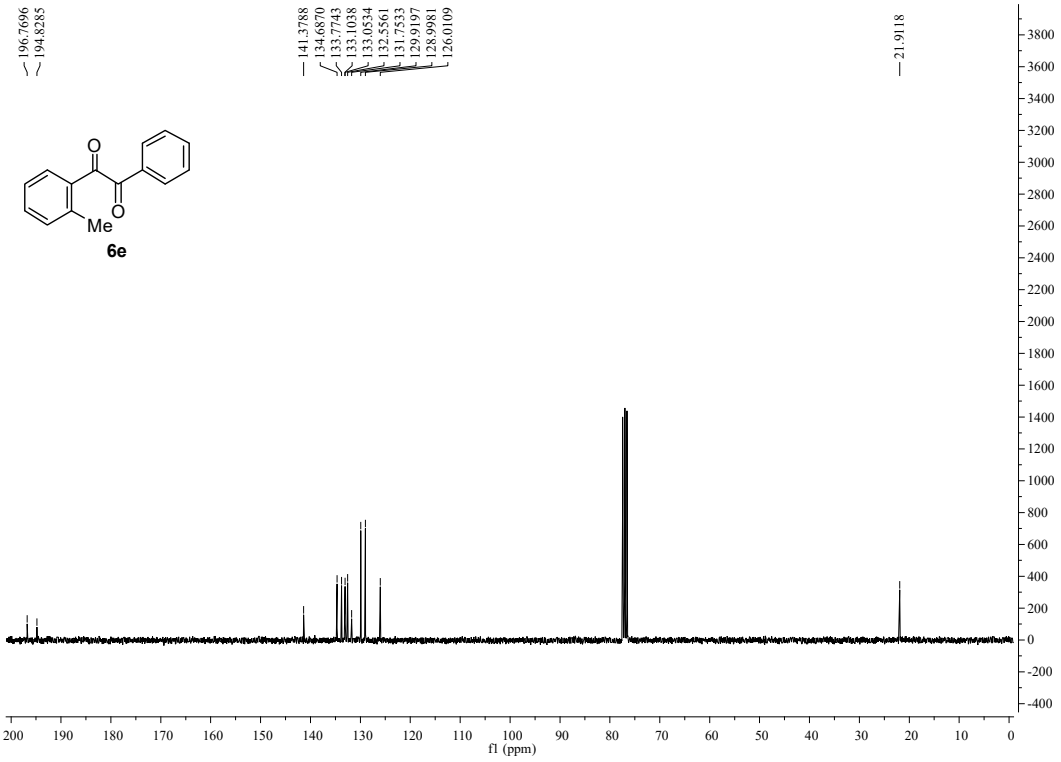
7.6499
7.6245
7.5991
7.5103
7.4856
7.4613
7.4377
7.3271
7.3022
7.2287
2.6773
O
O
Me
6e
1.98
1.98
3.02
1.05
1.30
3.00
f1 (ppm)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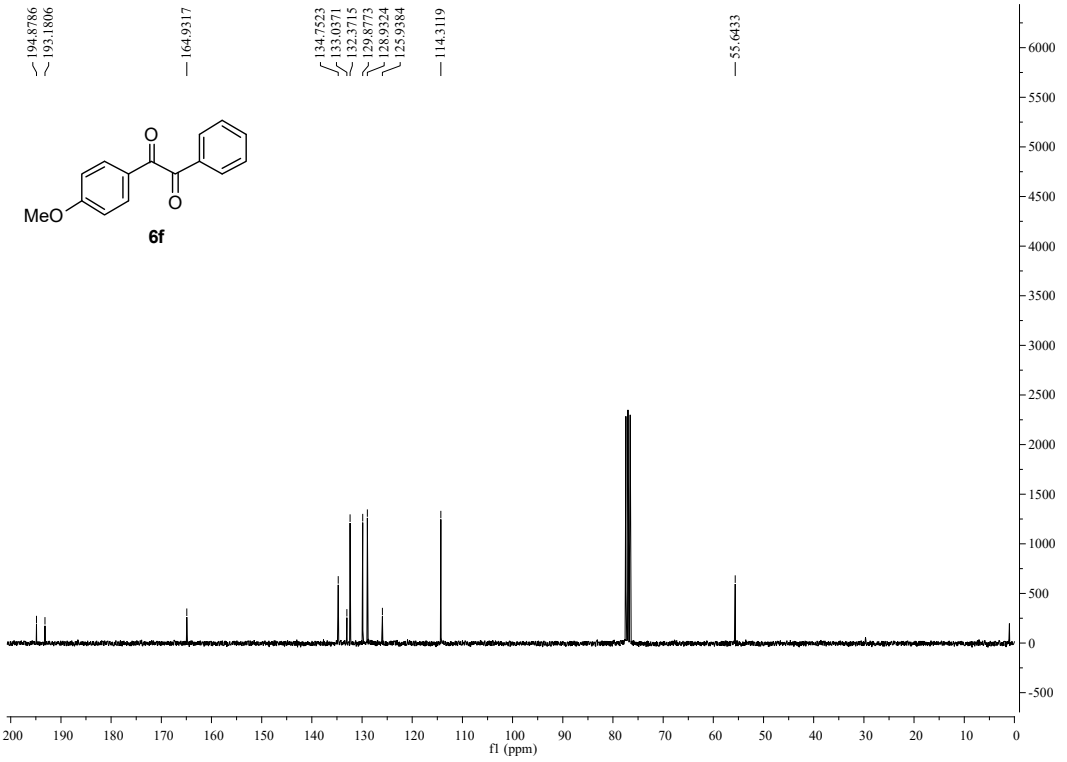
141.3788
134.6870
133.7743
133.1038
133.0534
132.5561
131.7533
129.9197
128.9981
126.0109
21.9118
O
O
Me
6e
f1 (ppm)


7.9801
7.9569
7.9320
7.6500
7.5280
7.5031
7.4787
6.9891
6.9607
3.8843
MeO
6f
3.91
1.05
2.00
1.99
3.00
f1 (ppm)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134.7523
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132.3715
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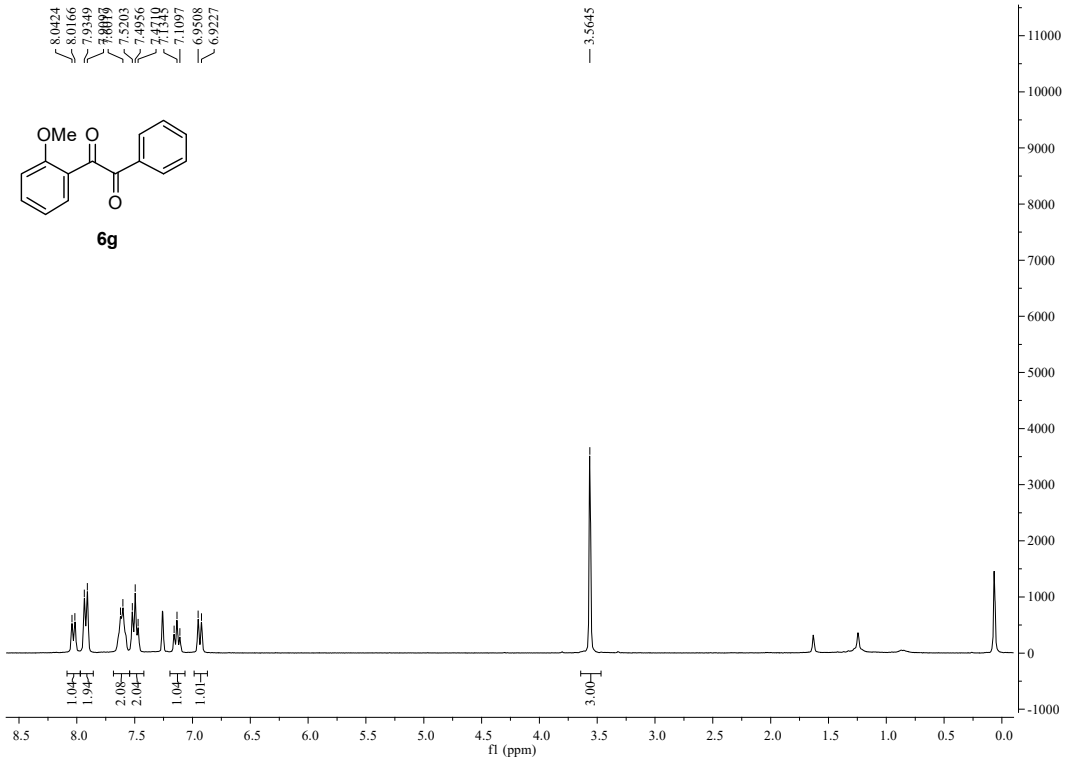
128.9324
125.9384
114.3119
55.6433
MeO
6f
f1 (ppm)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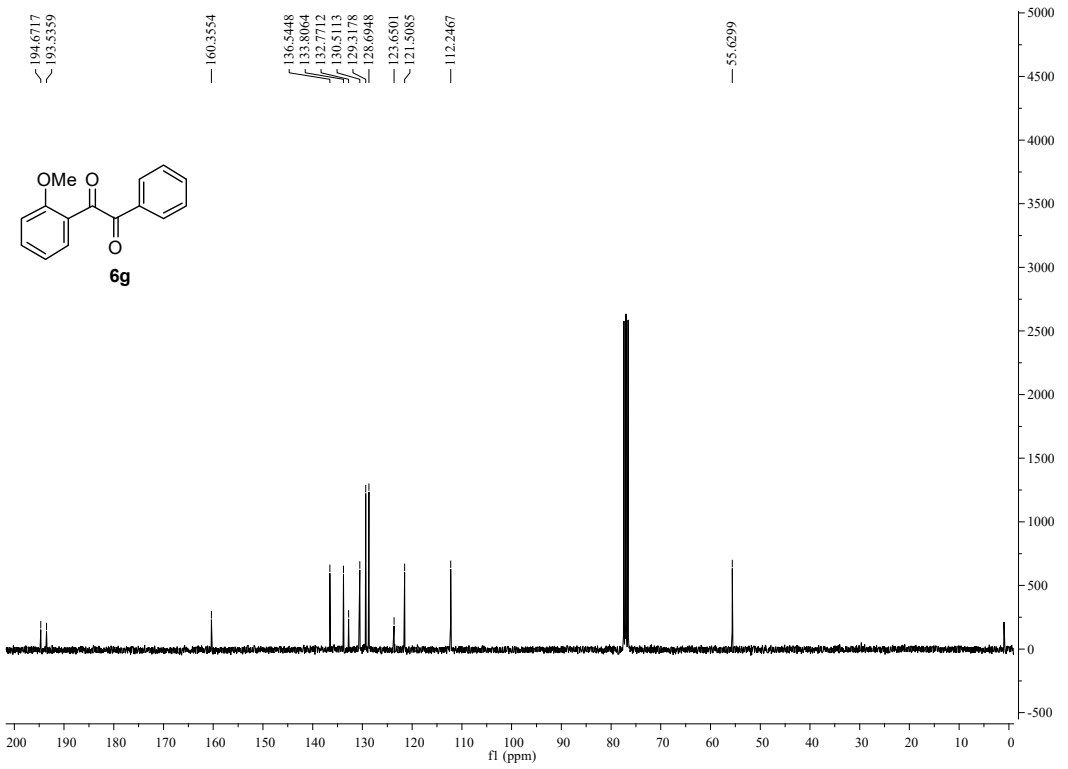
8.0166
7.9349
7.5203
7.4956
7.4710
7.1345
7.1097
6.9508
6.9227
3.5645
OMe
O
O
6g
1.04
1.94
2.08
2.04
1.04
1.01
3.00
f1 (ppm)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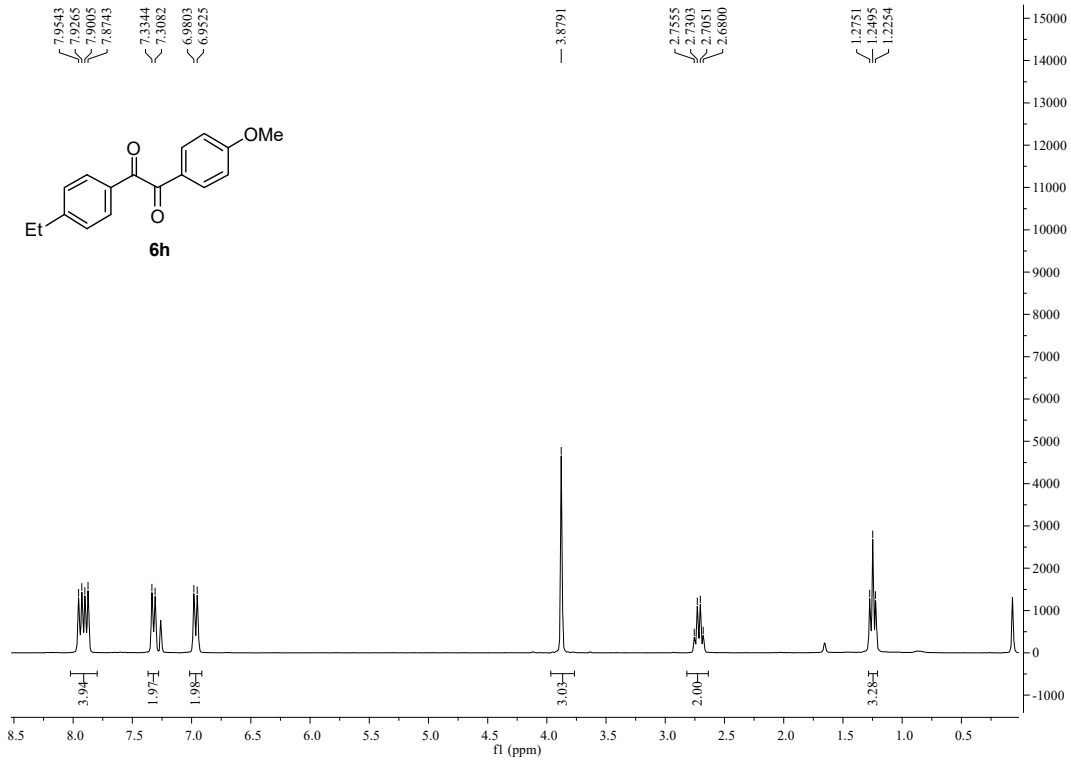
160.3554
136.5448
133.8064
132.7712
130.5113
129.3178
128.6948
123.6501
121.5085
112.2467
55.6299
OMe
O
O
6g
f1 (ppm)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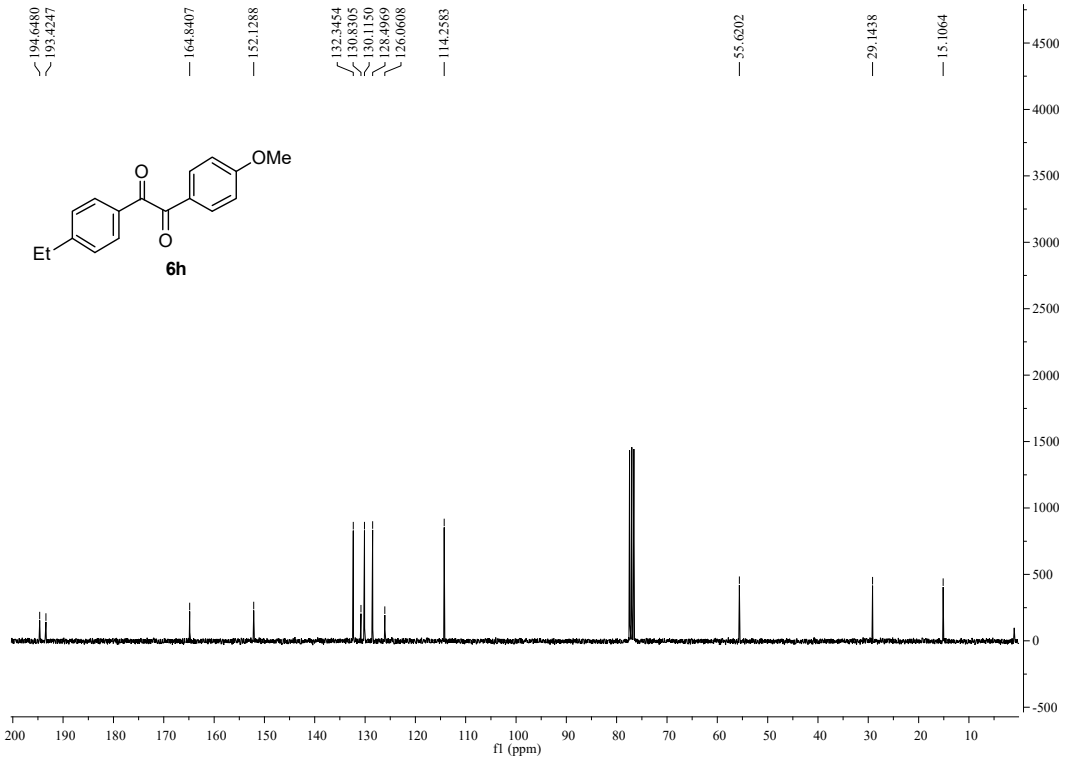
7.9265
7.9005
7.8743
7.3344
7.3082
6.9803
6.9525
3.8791
2.7555
2.7303
2.7051
2.6800
1.2751
1.2495
1.2254
OMe
O
O
Et
6h
3.94
1.97
1.98
3.03
2.00
3.28
f1 (ppm)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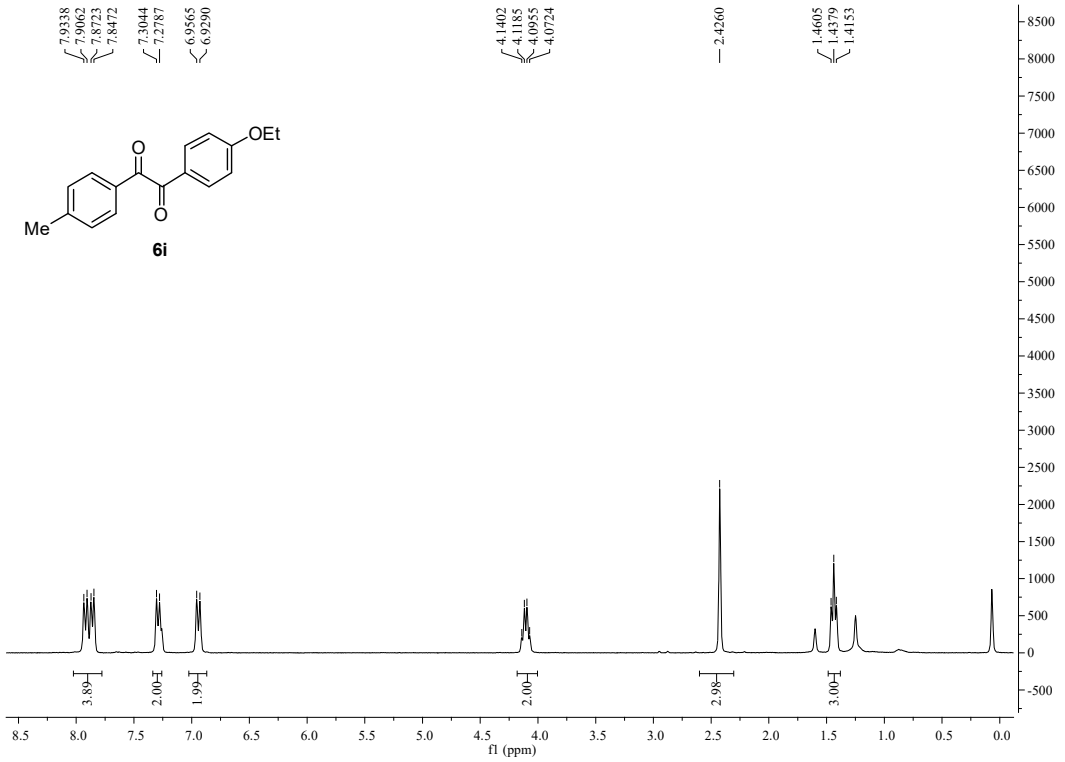
193.4247
164.8407
152.1288
132.3454
130.8305
130.1150
128.4969
126.0608
114.2583
55.6202
29.1438
15.1064
OMe
O
O
Et
6h
f1 (ppm)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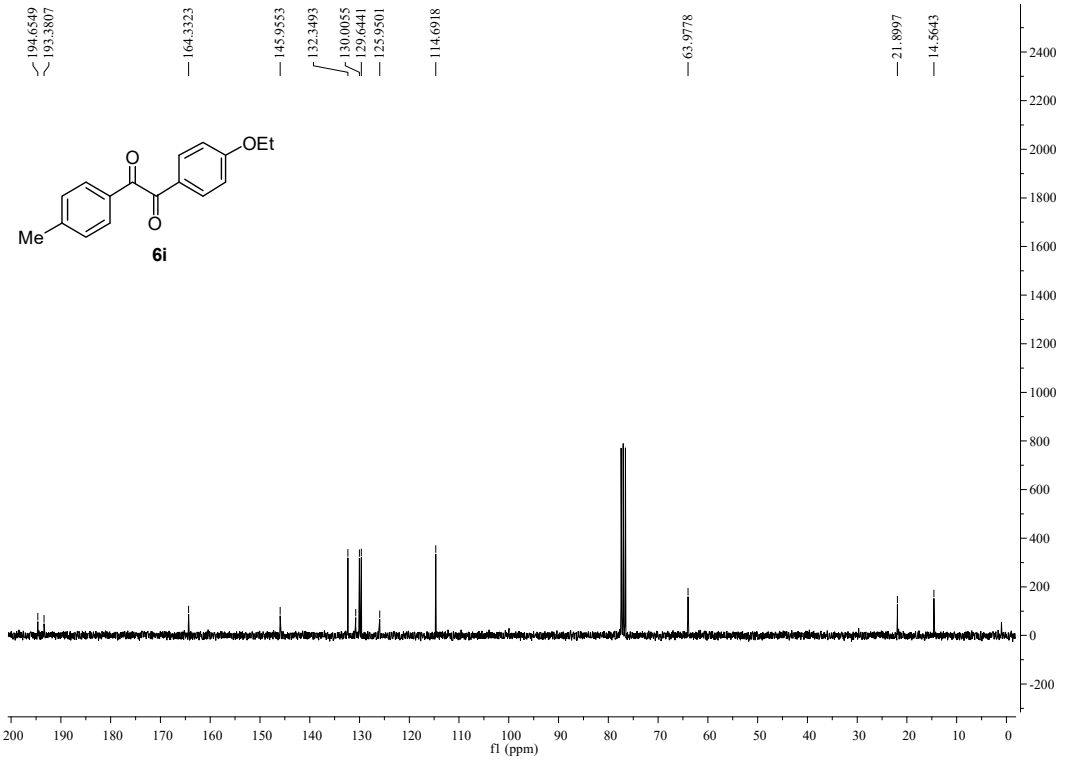
7.8723
7.8472
7.3044
7.2787
6.9565
6.9290
4.1402
4.1185
4.0955
4.0724
2.4260
1.4605
1.4379
1.4153
OEt
O
O
Me
6i
3.89
2.00
1.99
2.00
2.98
3.00
fl (ppm)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130.0055
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125.9501
114.6918
63.9778
21.8997
14.5643
OEt
O
O
Me
6i
fl (ppm)

11. Gaussian archive files

Chlorostyrene

α-chlorostyrene

16

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C -4.7212755314 -4.0234029743 -2.0334508391

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H -3.0470717486 -2.765686904 -2.1477628245

C -4.4922098195 -4.8294575834 -3.2438206037

C -3.9519719139 -6.3335842702 -5.5433057119

C -3.8625434619 -4.2438841693 -4.3488135491

C -4.8647229571 -6.1746279257 -3.3175096866

C -4.5912254287 -6.9202376947 -4.4565018848

C -3.5909637959 -4.9912250203 -5.4861154311

H -3.6094841787 -3.1863650148 -4.3205183704

H -5.3654429898 -6.6372126015 -2.4708304463

H -4.881166702 -7.9674175541 -4.4945257942

H -3.1081449087 -4.5183997546 -6.3379044554

H -3.74505757 -6.9175869025 -6.4366916483

Cl -6.1403689601 -4.4534560163 -1.0788472189

O2t

2

0 3

O 0.6690802635 -0.37854889 0.

O -0.5373048235 -0.37854889 0.

pdt1

17

0 1

C -2.5905648175 2.4968355966 -0.8775333903

H -3.630164677 2.8115684323 -1.0104974127

H -1.929356808 3.1199838435 -1.4811333685

C -2.3663874706 1.0473118813 -1.2808762721

C -3.2526722469 -0.0084121577 -0.7300490082

C -4.8816061278 -2.0765962608 0.1830647806

C -4.3423384207 0.2682831625 0.1010398264

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C -3.7965999301 -2.3605126233 -0.6432052432

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cpx1

11

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Cu -0.3611327963 0.2770481804 -2.1900014019

Cl 0.1014476902 2.2771738724 -3.3165223359

Cl 0.2503947176 -1.7609349535 -3.1637062718

Cl -0.9063511499 0.3467424035 0.0877366274

O 1.3837388753 0.3637008892 -1.6234380455

Cu 2.2898851002 -1.1262101688 -2.2011387079

Cu 1.4297117028 0.433169622 0.2111414034

Cu 2.1764689195 1.8696603594 -2.3140795601

Cl 3.6719876088 0.3833324791 -3.335449754

Cl 2.6649911667 -1.5508438813 0.0701838312

Cl 2.519856165 2.4861621975 -0.0817247849

cpx2

27

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Cu 0.8883331645 -0.9134453931 -1.3584883658

O 0.6555877944 0.1462704639 0.1721087932

Cu 0.8576009663 -0.7476197355 1.7814399196

Cu -0.8920920253 1.1288344164 0.5698312429

Cu 1.8731347711 1.5238422819 -0.3993441803

Cl -0.1979483198 0.8802287997 2.8487169076

Cl -0.8160872311 -1.7153363248 -2.285291919

Cl -0.190736787 2.6054712798 -0.9608441744

Cl 3.2492858183 3.1061259252 -0.1613611354

Cl 2.9683602583 -0.2164930069 -1.5080850343

C -4.0224110588 -2.4351886494 -0.6093167382

C -3.2221222314 -1.6060428503 0.0537568649

H -3.943830655 -3.510991565 -0.4999563841

H -4.7846853131 -2.043596509 -1.276771702

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Cl -2.0362150111 -2.2704848503 1.1707932086

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C -3.5748772413 0.4737744296 -1.2714710341

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H -2.7638065476 2.6946013156 1.7979534027

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TS1

27

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Cu -2.321403 -0.652546 -0.404588

Cl -0.037484 3.732041 -0.524838

Cl 2.2817 -2.484421 -1.194078

Cl -2.828394 -1.010528 1.863324

Cl -2.858709 1.354358 -1.271295

Cl -1.356357 -2.55509 -1.364866

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C 3.113162 -0.236303 0.672952

H 4.448006 -1.660455 -0.192031

H 3.328027 -2.33584 1.08879

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Cl 3.911584 1.023851 -0.202924

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C 1.327762 -0.944161 2.245598

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H 2.182246 2.243375 1.318306

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H 1.579687 -1.987587 2.073384

C 0.058754 0.696935 3.489926

H 0.344725 2.742858 2.859319

H 0.08716 -1.429993 3.973352

H -0.686233 0.943567 4.241252

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cpx3

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Cu 0.8609112039 0.6560216449 1.8280506912

Cu 1.2765504823 0.487779914 -1.5504739782

Cu 2.0162011246 -1.4580435617 0.0625316429

Cl 1.1171604115 2.4512756266 2.9416437794

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H -4.2197644795 0.502358825 -1.9771127278

H -2.7433112791 0.2091163049 -2.9503890093

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Cl -3.4296954736 2.1941142861 0.013238001

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C -0.3496177913 1.3305060448 -2.5077911613

C 0.8043194296 3.2331883312 -0.8306827622

H -1.0500528716 3.2565713196 0.2429792084

C 0.8985291848 1.8919451848 -2.8642510287

H -0.8112382044 0.6484955342 -3.2181249075

C 1.5144757833 2.7788572724 -1.947237868

H 1.2825450692 3.9066955524 -0.1245849812

H 1.359874119 1.6718854094 -3.8243052587

H 2.5129943324 3.1547352059 -2.1516634611

Cl -1.4861633405 0.0215294508 2.0164563475

cpx4

29

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O 0.6131508928 0.0408716934 0.2413227944

O -1.3860932642 -3.1292805869 0.4973396814

Cu 1.0462439516 -0.0384634687 2.0432861671

Cu 0.2042589432 1.8083847584 -0.2043592638

Cu 2.1285093866 -0.3125389338 -0.9031488754

Cl 0.7049489054 1.9472944672 2.7750541016

Cl -2.8492228045 -1.6936402749 -2.0822437215

Cl 2.1707430438 2.1142479183 -1.1549147117

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C -3.9816396062 -0.8115136995 -1.0050802922

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H -2.5735239178 0.8161311278 -2.6474604807

C -0.7671969197 3.3420615716 -1.2186872368

H -0.8394024759 3.930436316 0.8788983881

H -1.0537775699 2.6387472319 -3.2577238198

H -0.1576105492 4.1864723406 -1.5270533824

Cl 1.4409385046 -2.1317525286 2.2155192003

TS2

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Cu 0.286451655 -1.248451569 -0.7738726494

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O -0.9712965732 -2.6286695495 -1.1738646565

Cu 1.0549299621 -0.7681139927 1.9118722869

Cu -0.3929439284 1.6135820305 0.9133636883

Cu 2.1996034939 1.0435939221 -0.5599710147

Cl 0.3062589509 0.52539074 3.4579679421

Cl -1.8460436015 -0.4610450221 -3.1920244737

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Cl 4.1659991914 1.7362565293 -0.9358351781

Cl 1.7398435789 -0.444297285 -2.2749932558

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C -3.1689588553 -1.1282615354 -2.1868323828

C -3.1045058235 -0.7477470268 -0.7451736188

H -3.0855285727 -2.2190764084 -2.2495557687

H -4.1249863202 -0.8223906915 -2.6277353551

C -2.7263368054 0.5279808235 -0.2064888103

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C -2.468266561 0.6513306511 1.1866734814

C -2.6095609745 1.6891102752 -1.0146460094

C -2.2507299148 1.9023987861 1.7774907918

H -2.5384991828 -0.2275677093 1.8238862299

C -2.2655938173 2.8977114195 -0.450798078

H -2.8083129771 1.6341717484 -2.0787870666

C -2.0288151882 3.0114995541 0.9414718677

H -2.1501710293 1.9843861284 2.856002996

H -2.1550838576 3.7763419893 -1.0791038182

H -1.7945911942 3.9795676069 1.3743359996

Cl 1.6914970015 -2.6439750055 1.127636508

cpx5

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Cu 0.3400889278 -1.4787652592 -0.6311803198

O 1.035599097 -0.0355397409 0.4268642865

O -1.0903288139 -2.6244444663 -0.9063197755

Cu 1.3781669156 -1.0012052217 1.9576377928

Cu -0.1642812063 1.2373876868 1.1267676581

Cu 2.1347207387 0.7917954199 -0.9115374981

Cl 0.601684291 0.6095871033 3.2654033588

Cl -1.1932634346 0.0111512858 -2.8099371419

Cl 0.4818307055 2.6077152793 -0.466457519

Cl 3.6816634566 1.9066733198 -1.8226448028

Cl 2.1218725887 -1.2530368116 -1.9778501169

O -1.6281487819 -1.5610381399 -0.0864075852

C -2.6326254261 -0.8730203589 -2.203670702

C -2.6865456189 -0.8586876198 -0.6905068305

H -2.5545591736 -1.9058898927 -2.542731781

H -3.5257857226 -0.4054680185 -2.621446895

C -2.7096475682 0.4998765297 -0.0308896903

Cl -4.2428471232 -1.7343756001 -0.2762135002

C -2.275450962 0.6221541494 1.2994204151

C -3.1305720658 1.6395832288 -0.7092529581

C -2.1813090234 1.8924474029 1.8972387728

H -2.0966184294 -0.2744995773 1.893562331

C -3.0729203509 2.8941238873 -0.104927193

H -3.4832448453 1.5687924029 -1.7341809289

C -2.5889455672 3.0296946228 1.1862108477

H -1.9421091152 1.9662940474 2.9561840392

H -3.3911061354 3.7698743598 -0.6623230769

H -2.522357728 4.0093173633 1.6501416704

Cl 1.7061433709 -3.0301793821 1.5586591428

TS3

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Cu 0.8243774624 -0.9154658683 -1.2975047386

O 1.1365592685 -0.2069749239 0.4368603704

O -0.6662961076 -1.8812071861 -1.8404532339

Cu 1.5370492875 -1.8027042792 1.2699697484

Cu -0.5211326506 0.2015292668 1.2563668826

Cu 2.026961685 1.4399781401 -0.0075262437

Cl 0.0293105523 -1.475042377 2.8506038233

Cl -1.1796434168 1.3033536311 -2.6238159901

Cl 0.0170519037 2.3442070469 0.9906639852

Cl 3.3822650219 3.0577234771 0.0966457143

Cl 2.3496961639 0.4559474353 -2.1101589556

O -1.3279971975 -1.1584641659 -0.7730343085

C -2.4663206223 0.0544354466 -2.5387670128

C -2.5310743643 -0.5683899703 -1.1612894486

H -2.2176422347 -0.7231986487 -3.2614957996

H -3.4218051058 0.5150715241 -2.7984842608

C -2.868129723 0.3323084348 0.0017811792

Cl -3.8299503724 -1.8593127093 -1.2970957396

C -2.6331871493 -0.1729022572 1.3023484943

C -3.3345831327 1.6292980347 -0.1474145838

C -2.8140133058 0.6561419003 2.4182066172

H -2.4977477417 -1.2458833136 1.4410293461

C -3.5396293846 2.4330836125 0.9756560638

H -3.5106036844 2.0451643585 -1.1349725047

C -3.2570322566 1.9666689786 2.2511619072

H -2.639986577 0.2519528715 3.4130444569

H -3.8955922062 3.4502821824 0.8388468259

H -3.3893134608 2.6122587075 3.1138523617

Cl 2.621285349 -3.0019263492 -0.0679589561

cpx6

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Cu 1.066449154 -1.3495844724 -1.0822168507

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O -0.4952107173 -2.2519054147 -0.716452175

Cu 1.3462255576 -1.3780232287 1.6961199899

Cu -0.6648072017 0.4836706794 0.8740394637

Cu 2.0530249276 1.3722644761 -0.2630768488

Cl -0.1420238126 -0.6141083518 3.0964469931

Cl -0.9411668167 0.0879252923 -2.8646909299

Cl 0.0418929349 2.5385858912 0.3419363963

Cl 3.4689139771 2.9309552041 -0.4501170999

Cl 2.6552979619 -0.157882492 -2.0157298493

O -1.3324054769 -1.2544745632 -0.1308139908

C -2.2865705895 -0.9884585562 -2.3476941928

C -2.490652132 -0.9507227365 -0.8486351849

H -2.0199384789 -2.0033389732 -2.6426495024

H -3.1960075526 -0.6786298562 -2.8666555526

C -2.9152115706 0.3560121264 -0.2170526654

Cl -3.774245466 -2.2188147435 -0.535987238

C -2.831038006 0.4462358134 1.1943076252

C -3.3017395684 1.46950613 -0.9516217172

C -3.1208779612 1.6583420694 1.8326438328

H -2.7463263279 -0.4643419233 1.7880447035

C -3.5903250848 2.6647343059 -0.2967475858

H -3.3521760274 1.4315996814 -2.0358599072

C -3.4826811178 2.7716203143 1.0858619197

H -3.0544210581 1.7126584207 2.916437767

H -3.8797171681 3.5318697152 -0.8838529972

H -3.6884004159 3.7173231255 1.5778035837

Cl 2.6083781259 -2.809478403 0.7550888768

cpx7

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0 5

Cu -0.1436305167 -0.4131462514 -1.1514775958

Cl -1.0549122956 0.9803813383 -2.5571164812

Cl 1.9155893644 -0.7775725341 -2.3801472578

Cl -2.0050226683 -1.0782675501 3.213221423

O -1.3390124382 0.1038808958 0.2538268066

Cu -1.736698489 1.8892858296 0.5373864104

Cu -0.7729487525 -1.1366512479 1.532276206

Cu -2.857772105 -0.2998336472 -0.7505857893

Cl -3.8837284598 1.5554256803 -0.0509760967

Cl -0.0730771311 2.977594445 1.1863281801

Cl -2.4125880406 -2.3281384839 -1.2350206396

C 2.7981722821 -1.7591082903 -1.1263510955

H 3.8131715422 -1.8951883394 -1.5031148275

H 2.2701985103 -2.7096730518 -1.0567276302

C 2.8248006768 -1.0196942552 0.2068312489

C 3.7125773716 0.201459454 0.2121277663

C 5.3555680683 2.4505089969 0.0859202686

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H 5.5462799024 -0.9340369033 0.2662265039

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H 6.9968584893 1.054853451 0.1297616852

H 5.9974685875 3.3265740127 0.0418195627

Cl 3.4497645169 -2.3136583707 1.3601058478

O 1.5680461905 -0.6032069326 0.6196254798

O 0.567172606 -1.5787573597 0.2458859025

TS4

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0 5

Cu -0.5830584061 -0.8674635501 -0.7654190934

Cl -2.3508279535 -1.1659221033 -2.0794151923

Cl 1.1311500862 -1.7479866826 -1.9075119952

Cl -1.4911590205 1.6118849571 3.2570529384

O -1.5375585386 0.4173995451 0.2391514119

Cu -1.8957691235 2.1275597753 -0.3621909699

Cu -0.882320747 0.0719796075 1.9671554173

Cu -3.2429521935 -0.3311453824 0.1204818963

Cl -4.0889636304 1.774320636 -0.3021924171

Cl -0.0505624947 2.9568941673 -0.9400313176

Cl -2.938528299 -1.7997991754 1.6951800671

C 2.4065036909 -2.2793198289 -0.030163564

H 3.2113694006 -2.7015085591 -0.6183310499

H 1.6084397491 -2.910117662 0.3313499908

C 2.5373068507 -0.9092209837 0.4338335107

C 3.5554265268 0.0094896629 -0.0883786428

C 5.3880404598 1.7483412485 -1.2439692337

C 4.8707824814 -0.4133437687 -0.3173087001

C 3.1625560279 1.306902417 -0.4388642021

C 4.0836103028 2.1693702766 -1.0171142792

C 5.7796172094 0.4566899308 -0.893922502

H 5.1889231253 -1.4059306894 -0.0079938553

H 2.1356801135 1.6353246637 -0.2957284407

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H 6.8019687729 0.1310641043 -1.0635348599

H 6.1066752827 2.4264575388 -1.6968282306

Cl 3.4346607697 -2.2060708543 1.9503167616

O 1.4944846103 -0.2835284476 0.9389629519

O 0.3310231776 -1.1151329938 1.0300205518

cpx8

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Cu 0.2811077781 0.2891633971 1.3261615119

Cl 2.1942615055 0.4287196636 2.6223343052

Cl -1.4492080326 1.0069420733 2.4169314455

Cl 0.0137001405 -2.7771927264 -2.3978082069

O 1.4586206911 0.1388423673 -0.1412654061

Cu 1.8637929474 1.7481775972 -0.9625149645

Cu 0.864243798 -1.4675906793 -0.9681875476

Cu 3.1000363314 -0.2545532743 0.6288053702

Cl 4.0156727317 1.6707910348 -0.5764382375

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H -2.1449906081 -1.7503871615 1.9280977889

C -2.8443684813 -0.4774299177 0.3501142812

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C -5.7870280309 2.1835233449 -1.054233101

C -5.2033821994 0.2259324922 0.2120509405

C -3.4790623249 1.5180609605 -0.9336354565

C -4.4501093865 2.3917470508 -1.3877139017

C -6.1635609423 1.102338559 -0.2576861222

H -5.5008387988 -0.6294831328 0.8129367451

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H -4.1634488385 3.2450787047 -1.9948680111

H -7.2082870568 0.946925574 -0.0057134715

H -6.5451724508 2.8751013863 -1.4130218373

Cl -3.6844665774 -2.9529655328 0.5767477116

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O -0.6743549436 -1.1344365372 0.2936697963

TS5

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Cu -0.1288501015 0.3209399512 1.248850493

Cl -2.1206610795 0.0961348105 2.4733857112

Cl 1.4453456712 0.479861908 2.701897114

Cl -0.9697278654 3.463150554 -0.0672459867

O -1.1597523963 -0.3739656666 -0.2167708983

Cu -1.1806227829 -2.0350609973 -1.0322037785

Cu -1.2924105099 1.4286064977 -0.8433761435

Cu -2.9128798095 -0.3519520624 0.4206326124

Cl -3.2137381072 -2.5692144132 -0.3231849551

Cl 0.4768657236 -2.6868283353 -2.1278845254

Cl -3.4853011312 1.1555111038 -1.252113625

C 3.1413011812 2.0021008136 0.3041842173

H 3.9414910137 2.0162461362 1.0445994546

H 2.2769698125 2.5616279708 0.6568867598

C 2.752514912 0.5976395156 -0.0635947435

C 3.7221860231 -0.4843811484 -0.0161396152

C 5.5295597678 -2.591191131 0.0563189779

C 5.098728802 -0.2243166172 0.0747303016

C 3.2615355945 -1.8092193835 -0.0660723769

C 4.1644288244 -2.8564818596 -0.0263445824

C 5.9956282679 -1.2786016924 0.1039754842

H 5.4694553003 0.7973400536 0.0871330818

H 2.1941413898 -2.0015919883 -0.1304616484

H 3.8038938781 -3.8804639023 -0.0604981981

H 7.0617298157 -1.0796759409 0.163164366

H 6.2385512154 -3.4148198589 0.0857197715

Cl 3.7278981595 2.7728648599 -1.2109961478

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O 0.462294995 1.6962613057 -0.1876345528

TS3a

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Cu -0.375273211 -0.7317708375 0.57191497

Cl 1.1670809044 -3.0841841373 0.0477052832

Cl -0.1279194599 -0.2471533672 2.600556154

Cl -0.5186187613 2.2424191429 -1.857650788

O 1.2447556109 0.0427800224 -0.0004687413

Cu 2.2381553889 1.1251905536 1.1708031294

Cu 0.9295771635 0.711997637 -1.7327275935

Cu 2.4480943294 -1.3635302651 -0.2944410292

Cl 3.9780576604 -0.2722792998 1.0496774181

Cl 1.6741164643 3.0574531529 1.701147037

Cl 2.6077923277 -0.4184135943 -2.5680834501

C -2.1032118048 -1.4778296671 0.8188210849

H -2.5366570665 -1.3567408704 1.8075750394

H -1.846338683 -2.5134495547 0.5695683937

C -2.8096734941 -0.7700392988 -0.2427181355

C -3.8332965436 0.2257542526 -0.0673005757

C -5.7592811131 2.1788003497 0.3225179278

C -4.7447082015 0.1074765221 0.9980228598

C -3.8955354886 1.3284779454 -0.9387544546

C -4.8601006472 2.3011429464 -0.7323300244

C -5.7021319156 1.082479843 1.1875729628

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H -6.4125693248 0.9944420224 2.003996065

H -6.5108830014 2.9478489817 0.480918402

Cl -4.1066221272 -2.6365855384 -1.0907457475

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O -0.8255896693 -0.8703043328 -1.2512199695

cpx9

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0 5

Cu 0.3459227875 0.4112459023 -1.7938461586

Cl -1.0125375096 2.3279069002 1.5343511059

Cl 0.1261362298 -1.4265433936 -3.0747767539

Cl -1.8358292113 -3.8688403023 2.6188294424

O 0.5968204525 -1.2078758079 0.87713934

Cu 0.951624282 -1.777657493 -0.8576132621

Cu -0.535761145 -2.492402648 1.6268152126

Cu -0.1086939612 0.4102525326 1.257443064

Cl 2.5443777814 -0.2268814757 -1.3455420852

Cl 0.0037861301 -3.7026002279 -0.3145747881

Cl -1.0648371529 -0.5263316297 2.9369525641

C -3.1387760142 2.7304681336 -2.2243162038

H -4.2172347756 2.6125632193 -2.1052055386

H -2.8901981818 2.9338535277 -3.2683524403

C -2.3712716641 1.5125135609 -1.7734837394

C -2.961437793 0.5884378986 -0.8174963975

C -4.0160454966 -1.1836235524 1.0530347271

C -3.8932155576 1.038246186 0.1318859496

C -2.5955587134 -0.7683553774 -0.8440905942

C -3.135175449 -1.6512541198 0.0776342786

C -4.3969231664 0.1563260831 1.0750631803

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H -2.8786926859 -2.7085477279 0.0403513875

H -5.0797661339 0.5161266657 1.838855372

H -4.3961032672 -1.8765257311 1.7997768943

Cl -2.6089102816 4.1323424023 -1.2450844922

O -1.2469142075 1.3602895336 -2.2824378944

O 0.6315986163 1.2350661765 -0.158455372

cpx10

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Cu 0.9740656576 -0.6375155558 -3.9472573674

Cl 3.0420840074 3.2706997214 -3.6317871337

Cl 0.5564359912 -2.7600452786 -3.5611268576

Cl 0.2726792316 0.5121505862 1.5433049476

O 1.716354406 -0.1014434823 -2.1042415377

Cu 2.570139389 -1.7893341621 -2.182805496

Cu 1.2597227775 0.0442674717 -0.2773552802

Cu 2.4080804482 1.4560747876 -2.7681088756

Cl 3.8420549395 -1.3572420345 -3.8757637131

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C -2.9980936599 -1.8650446637 -0.9883067828

C -1.6235873676 0.0238408061 -1.5595878132

C -2.6137693695 -1.3342651199 -3.303269331

C -3.2138236892 -2.1259951305 -2.338935122

C -2.2072790722 -0.7871532442 -0.598740391

H -1.0321781864 0.884782265 -1.2477492915

H -2.7849479216 -1.5427165772 -4.3562589363

H -3.8473738745 -2.9547945299 -2.6414535063

H -2.0265323838 -0.5731861671 0.4519480369

H -3.4554995939 -2.4990678051 -0.2336713393

O 2.1300670772 0.7398008132 -4.4106135205

C -0.6424977552 -0.0330919199 -5.1475198382

H -1.0060981489 -1.0084540344 -5.4659105666

H -0.2322161659 0.6321290452 -5.9029665407

C -1.0692583315 0.4814708421 -3.9474888553

Cl -0.686878592 2.1480758406 -3.5985303973

TS6

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0 5

Cu -0.0675868787 -1.2168568072 0.8417772512

Cl -2.3329259856 0.0289091188 -2.9595941645

Cl 1.3374982385 -1.013916086 2.4167879212

Cl 1.6101387375 3.2778770229 1.3969610637

O 0.827123081 -0.1016297252 -0.4035394113

Cu 2.4027112099 -1.0625811059 -0.6330504751

Cu 1.432772235 1.6341550235 0.0451688445

Cu -0.7177875399 0.0890538879 -1.5469967009

Cl 1.7111272562 -3.0605406945 -0.8167724725

Cl 3.6260110929 0.718358414 -0.3457369853

Cl -0.1880065502 2.2966751691 -1.5142426701

C -2.748478343 0.1402446597 1.1240356062

C -2.8173698484 2.8764420127 0.5981108116

C -3.6766311819 0.6690650606 0.1955824021

C -1.8753828523 1.027540749 1.810143797

C -1.9162145477 2.378791051 1.5494635632

C -3.7061211453 2.0249151272 -0.0593665101

H -4.3143190306 -0.0032889306 -0.3704087157

H -1.149186516 0.6574154676 2.5311602579

H -1.2109333843 3.0451763292 2.0400043522

H -4.3841782589 2.4153756947 -0.81159678

H -2.8092171111 3.9368908753 0.3607900697

O -1.3380508369 -1.3317497721 -0.4542928188

C -1.4649106072 -1.881946895 1.9902781459

H -1.2879862523 -1.4608155507 2.98060406

H -1.4636594949 -2.9715298683 1.9837533132

C -2.5660702936 -1.2832271482 1.2529245813

Cl -3.8078841922 -2.3334850794 0.7328226632

cpx11

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Cu -0.2582408216 -1.4148693643 -0.8532293706

Cl 2.4456075725 -0.2970239018 2.8442758853

Cl -1.6299075061 -1.1185350888 -2.4265754886

Cl -0.8094222017 3.1907697031 -1.375794391

O -0.8795752359 -0.1678288853 0.5129358502

Cu -2.5913708632 -0.8496135232 0.6997682672

Cu -1.2054610804 1.626127041 0.1188649763

Cu 0.7443870249 -0.1175634631 1.5308893661

Cl -2.2769216777 -2.9215388429 0.9464888319

Cl -3.4994928882 1.1042481586 0.2179167716

Cl 0.2310311585 2.1208218701 1.814605948

C 2.2630433411 0.0987244197 -1.1277083382

C 2.4678034797 2.9139492387 -1.113538902

C 3.0505734465 0.7856339909 -0.1591079587

C 1.6272783837 0.8307577088 -2.1086506084

C 1.7432158996 2.2374435664 -2.1242128742

C 3.1174323274 2.1844087058 -0.141846979

H 3.6146677257 0.2083207039 0.57018861

H 1.0167117424 0.3569637279 -2.8734035175

H 1.3376689189 2.7948203636 -2.962555049

H 3.6855723774 2.6762073187 0.6418624317

H 2.5095452587 3.9989242683 -1.1246707592

O 1.2483852059 -1.5642026669 0.2221760607

C 1.1621295142 -2.0838564078 -1.924569944

H 1.1259091218 -1.7542988584 -2.9599904574

H 1.1676959588 -3.1665375432 -1.791983808

C 2.0316584859 -1.3879423095 -0.9267252982

Cl 3.648872331 -2.2102969301 -0.7539582551

TS7

28

0 5

Cu 0.9720475752 -1.4493982398 -0.5166435243

Cl 1.189876747 1.5476387057 3.1449206576

Cl 0.5097329242 -2.2920945961 -2.4004870215

Cl -3.1909359864 0.9381359583 -2.1149373386

O -0.5822221868 -0.6784676902 0.3026899258

Cu -1.218175775 -2.3760088306 0.7288024749

Cu -2.0529383123 0.1986227574 -0.4977809943

Cu 0.2455600958 0.6313410419 1.4632956512

Cl 0.6362951916 -3.3766944407 1.1454253275

Cl -3.1960889054 -2.0636033953 -0.0098552053

Cl -1.7582949949 1.6968718714 1.2073028115

C 1.5836940538 1.6800479163 -0.8762374011

C -0.0657809971 3.8813146603 -1.3110855004

C 1.6767927946 2.8002481103 -0.0454905943

C 0.6598876168 1.6674442974 -1.9259409962

C -0.159989142 2.7710441819 -2.1418263035

C 0.8519515065 3.8943313784 -0.2650086609

H 2.3857187035 2.80616518 0.779359376

H 0.5534007544 0.8021922466 -2.5810943056

H -0.8902108114 2.7439274507 -2.9454106306

H 0.9220292497 4.7557048994 0.3930248441

H -0.7170150388 4.7352119654 -1.4749264785

O 1.9037942463 -0.2088582825 0.5768980858

C 2.5586759578 -0.5828728314 -1.5760975134

H 2.4464202845 -0.3519469823 -2.6322150265

H 3.2142915627 -1.419637954 -1.322519445

C 2.3732836565 0.4526192061 -0.5277403423

Cl 4.1821732294 0.8788484156 -0.3471618723

cpx1a

27

0 5

Cu -0.2741326135 -0.5430459433 -0.6181601964

Cl -0.0157739909 1.3359037309 -2.1484992846

Cl 0.8447131928 -2.6732419934 -0.7276011683

Cl -0.5834215759 0.3004538868 1.8671232384

O 1.4480468337 0.0162232291 -0.1161560343

Cu 2.6760706125 -1.3489530879 -0.2342777277

Cu 1.6125882569 0.6530852688 1.6054048737

Cu 2.094154028 1.3669647358 -1.1843899939

Cl 3.7530647243 -0.1156304826 -1.907478187

Cl 3.3047660308 -0.9532884828 1.9616253801

Cl 2.5180000975 2.6490131634 0.6901839337

C -2.0025660499 -1.2223801133 -1.5172123633

H -1.7638135208 -2.253236811 -1.7662691249

H -2.0822794559 -0.5293736299 -2.3512057586

C -2.7364386251 -0.9828978651 -0.3785070026

C -3.4090157658 0.2627774258 -0.0313677698

C -4.6497890985 2.6855403453 0.5999313748

C -3.934927547 0.4827288224 1.2505881328

C -3.5183822657 1.2830850611 -0.9933791376

C -4.1322563957 2.4819066571 -0.6768598774

C -4.5499173588 1.6840942218 1.5603097153

H -3.8382901859 -0.2851902302 2.0117121801

H -3.1235002897 1.1438701972 -1.9955975262

H -4.2085399302 3.2607875702 -1.4299968621

H -4.9450470191 1.8427337389 2.5594973785

H -5.1305159279 3.628831418 0.8459762675

Cl -2.8743831601 -2.304822833 0.7359395397

TS1a

29

0 5

Cu -1.1232120203 -0.9066134183 0.1070631902

Cl 0.7495586007 -3.1721435443 0.3461808889

Cl -1.8634619097 -0.9557763218 2.1587978005

Cl 0.2931519787 2.4213494476 -1.8239474679

O 0.4536514628 -0.0144324361 0.6314493824

Cu 0.3340847762 0.8315767211 2.3057440526

Cu 1.3074156172 0.8953321113 -0.7791967723

Cu 1.6971853754 -1.3595721572 1.0478454806

Cl 1.9590859758 -0.4191445404 3.1693696266

Cl -0.705388895 2.6703301207 2.3190466297

Cl 3.2183412778 -0.1197020304 -0.4234597299

C -2.7390982757 -1.5927860143 -0.6328757888

H -3.4912096791 -1.6474903931 0.1685820686

H -2.5168333041 -2.6058463223 -0.9823891932

C -3.2561511452 -0.745330542 -1.7031825519

C -3.3069987292 0.6709835819 -1.6887605068

C -3.2452596394 3.4570375004 -1.6382710533

C -2.9083000077 1.3674781637 -0.5173906399

C -3.6771842691 1.417773556 -2.8358670358

C -3.6396392623 2.7927884346 -2.8054731838

C -2.8905600416 2.7460096889 -0.4934045771

H -2.6389293192 0.8217652267 0.3843449633

H -3.955825091 0.8999579972 -3.7483507843

H -3.8993994747 3.3615162814 -3.6929536238

H -2.560685636 3.2545543711 0.4086826738

H -3.2019504328 4.5430371302 -1.6288271499

Cl -4.033650475 -1.5815914223 -2.9847047279

O -1.0306629669 -0.8106849656 -2.7016250803

O -0.3608374905 -0.790067225 -1.6379568903

cpx2a

29

0 5

Cu -1.121968803 -0.8720641111 0.1664397612

Cl 0.7133176951 -3.0933867979 0.1061876105

Cl -1.8539720322 -1.0007205179 2.1495757736

Cl 0.2126936899 2.1789686535 -1.9683592023

O 0.5238608894 -0.0308110179 0.6078603664

Cu 0.5164555705 0.8561393394 2.2597216168

Cu 1.3586972546 0.8481442803 -0.8191780307

Cu 1.7594319177 -1.3948534494 0.9704097392

Cl 2.0324863223 -0.5308377408 3.1113404767

Cl -0.5178945558 2.6791389944 2.2263297907

Cl 3.2920541639 -0.1177905886 -0.4598499869

C -2.7370273641 -1.5564048549 -0.52934377

H -3.6002234272 -1.4575627819 0.1275811733

H -2.4901832975 -2.605312564 -0.7267940538

C -2.8743251093 -0.7523857578 -1.7915590461

C -3.1309377262 0.7156309015 -1.7011413456

C -3.399213041 3.4844213275 -1.5986955895

C -3.0276048475 1.386661393 -0.4800835247

C -3.3503302609 1.4442074264 -2.8766344421

C -3.4936449463 2.8203955629 -2.8202924202

C -3.1616436667 2.7686928488 -0.4316638106

H -2.8518187701 0.8487279891 0.4488791374

H -3.4061005042 0.926965349 -3.8314973299

H -3.6664623082 3.3808888344 -3.7345968187

H -3.0632951446 3.275886936 0.524035792

H -3.5002381287 4.5656091576 -1.5600464996

Cl -4.0309463684 -1.6015179016 -2.862070321

O -1.5735701446 -0.912488062 -2.5197575915

O -0.5903600571 -0.8240358481 -1.6583264548

TS2a

29

0 5

Cu 0.2480630278 -1.1044494869 -0.7933320987

Cl -1.8593747083 -2.8906276217 0.2794933439

Cl -0.3682898676 -0.8887223529 -2.7966498109

Cl 1.4761889064 1.4947045464 2.58009058

O -1.0085676615 0.0734709182 0.0157795665

Cu -1.8367293874 1.4195352464 -0.9664092411

Cu -0.1558819779 0.540360847 1.6275700364

Cu -2.5247940662 -0.8521357158 0.5951289709

Cl -3.851452421 0.5417992598 -0.7843510882

Cl -0.4743908055 3.0037077171 -1.2244003045

Cl -2.1331173094 0.3776208784 2.6506756378

C 1.8358259718 -2.0079986522 -1.2622540099

H 2.1407168203 -1.8988224292 -2.3020814712

H 1.6257123458 -3.0511326871 -1.0025818765

C 2.7853337867 -1.3713568867 -0.2830023456

C 3.0972611218 0.0894743124 -0.4169930203

C 3.5989819615 2.837670333 -0.4474401372

C 2.5696064957 0.8767751464 -1.4327298934

C 3.8579885916 0.688246074 0.6058065811

C 4.1122738343 2.0584861843 0.578574331

C 2.8289105505 2.2483626578 -1.4497634776

H 1.9597821241 0.4494313802 -2.2254576778

H 4.2476781444 0.0746825743 1.4145088552

H 4.6916707822 2.5102472303 1.3783000216

H 2.4162683603 2.8539948833 -2.251300976

H 3.7834224017 3.9077558741 -0.4661894361

Cl 4.2899069242 -2.3563243675 -0.2355039344

O 2.2192569174 -1.5564698195 1.0411525583

O 0.9018851364 -1.2256970437 0.9609063169

cpx3a

29

0 5

Cu 0.236616 -1.407659 -0.617035

Cl -2.927822 -2.587255 0.978155

Cl -0.281104 -1.540611 -2.652559

Cl 1.481345 1.774145 2.323195

O -1.063434 -0.133144 -0.081514

Cu -1.663259 1.128793 -1.308759

Cu -0.111223 0.590264 1.39241

Cu -2.68889 -0.489673 0.764075

Cl -3.770581 0.662607 -1.236356

Cl -0.034987 2.488929 -1.602799

Cl -2.116152 1.320626 2.157678

C 1.892371 -2.28881 -0.840368

H 2.24881 -2.332895 -1.868964

H 1.735973 -3.288616 -0.423262

C 2.730307 -1.450124 0.088552

C 2.974103 -0.01089 -0.299045

C 3.460636 2.718259 -0.849389

C 2.653046 0.510506 -1.53177

C 3.533575 0.842337 0.681673

C 3.777866 2.206397 0.391549

C 2.89412 1.877374 -1.80929

H 2.195519 -0.102062 -2.306239

H 3.847382 0.421088 1.633543

H 4.206267 2.837481 1.164622

H 2.643281 2.262703 -2.793273

H 3.633168 3.765079 -1.077202

Cl 4.33592 -2.261769 0.304928

O 2.1419 -1.506802 1.371278

O 0.783638 -1.158364 1.13038

cpx6a

29

0 5

Cu 1.1073168533 -0.9616559052 -1.5001934792

O 1.2695780145 -0.1896592784 0.2080280264

O -0.7206830561 -0.7380032697 -1.5973431141

Cu 1.09251491 -1.662984444 1.3211566517

Cu -0.3455793726 0.6667601484 0.6521283808

Cu 2.6288228182 1.0966243584 -0.1259913291

Cl 0.1935970463 -0.6383043842 2.9910668636

Cl -5.0761852711 -0.8671607694 -1.4460692004

Cl 0.7998621834 2.5652329142 0.2820762871

Cl 4.3476889072 2.3030648297 0.0798718049

Cl 3.1233781308 -0.3230164689 -2.0440164124

O -1.2327858545 -1.0421797403 -0.2731414857

C -3.3226265383 -1.1933358634 -1.4842220486

C -2.633585077 -0.6940704815 -0.229224355

H -3.1655662485 -2.2716911325 -1.5608010078

H -2.8976962281 -0.7138155026 -2.3660457235

C -2.6798601935 0.7949017308 0.0541577637

Cl -3.2121599879 -1.6463911387 1.1778600165

C -2.308905863 1.2568354001 1.340717336

C -2.9278842814 1.7241397906 -0.954912652

C -2.2636721497 2.6341071595 1.601552114

H -2.2873471943 0.5597892175 2.177995699

C -2.8591202458 3.0860347025 -0.6791281933

H -3.1901773504 1.3954636324 -1.9556169314

C -2.5256124619 3.5463502922 0.5922913226

H -2.0006278166 2.9725627076 2.6000092591

H -3.0618773968 3.7976133883 -1.4747704876

H -2.4718490181 4.6124376558 0.7905897184

Cl 1.4888807417 -3.2719305489 -0.0336348238

TS4a

29

0 5

Cu 1.1687267207 -1.5587900359 -1.0658823072

O 1.2449319317 -0.1936187673 0.1913229565

O -0.838822877 -1.8522874412 -0.8279142329

Cu 1.5272713874 -1.2761148609 1.6712712351

Cu -0.40639898 0.5920952892 0.7335542709

Cu 2.2469884251 1.2047886498 -0.6692594804

Cl 0.5816539567 -0.1828585045 3.231818713

Cl -4.357505087 -0.4275221388 -2.5775120154

Cl 0.5544934585 2.5451073314 0.2150750891

Cl 3.8508725729 2.49367449 -1.1134683212

Cl 2.2053437176 -0.3485533102 -2.5599398116

O -1.2826704183 -1.2479969075 0.4026439261

C -2.139252598 -1.2617154583 -1.5778388639

C -2.5877659911 -0.7924449843 -0.2064092728

H -2.627043829 -2.1215915773 -2.0200111172

H -1.7750521179 -0.5152596256 -2.2827151951

C -2.6500089655 0.6684280967 0.1670844028

Cl -3.8706536276 -1.7410287741 0.5341856649

C -2.3522020768 0.9655056778 1.5270206966

C -2.9643958659 1.7015748486 -0.7166060591

C -2.4128896063 2.2922102059 1.9790236388

H -2.2999764371 0.1588060396 2.2615087265

C -3.0001716996 3.008567935 -0.2417472899

H -3.2362578504 1.4527296574 -1.7423986056

C -2.7269296944 3.3094751949 1.0929226916

H -2.1990575396 2.5051471918 3.0229198256

H -3.2497519387 3.8086761761 -0.9330493425

H -2.7640069095 4.338818074 1.4371029769

Cl 2.0932609395 -3.0655464722 0.5471681004

Methylstyrene

α-methylstyrene

19

0 1

C -1.3436294194 0.4648959563 0.0963121672

C -1.8375605518 1.673082589 0.3898580887

H -2.9099937562 1.8521504272 0.4013235662

H -1.2012010109 2.5150204496 0.6498927362

C 0.1127740828 0.2039212518 0.0495449639

C 2.8816799554 -0.2950835383 -0.0174509278

C 1.0271005649 1.2309301856 -0.2206000017

C 0.6209687238 -1.0830395489 0.2615455578

C 1.9887221379 -1.3292456766 0.2350721541

C 2.3923411336 0.9873604849 -0.2491577212

H 0.6559130179 2.2301098321 -0.4384224674

H -0.0603544306 -1.9063787617 0.4639555471

H 2.3569142137 -2.3372802226 0.4119838588

H 3.0794858046 1.8018766103 -0.4670280355

H 3.9515302237 -0.4873098255 -0.0444013559

C -2.2648257591 -0.6874582272 -0.1802734231

H -2.0003235564 -1.1996478819 -1.1137138958

H -2.2191269024 -1.4401103305 0.6178229367

H -3.3029512316 -0.3502547336 -0.2512534183

ketone

17

0 1

C -0.654087723 -0.3498643254 0.5215171748

C 0.1832037915 -1.0075777004 -0.5460319132

H 1.2209863301 -1.0353518577 -0.2097537333

H -0.1625932625 -2.0289048546 -0.7444987338

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O -0.1476136481 0.0486830509 1.5535023272

C -2.1195887476 -0.1993280502 0.2816909463

C -2.7420496272 -0.64224378 -0.8879808953

C -2.8886009635 0.411468925 1.2763806514

C -4.1110254932 -0.4769163267 -1.0599735484

H -2.1594751766 -1.1198378353 -1.6728085903

C -4.2543263043 0.5767198387 1.1054491702

H -2.3815724114 0.7476382851 2.1773310412

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H -4.5892005357 -0.8238708334 -1.9726567809

H -4.846553268 1.0527076704 1.8831984864

H -5.9385821472 0.2613438084 -0.1991077159

aldehyde

4

0 1

C -0.7103913817 -0.2888844706 0.5102195625

O -0.1794139481 0.1384651338 1.4982995243

H -0.1455517348 -0.8004274829 -0.3017900032

H -1.8066415479 -0.2050396255 0.33334325

cpx2b

30

0 5

Cu 0.6252869856 1.0806216534 1.538443797

O 0.6204587357 0.1985973059 -0.1157631958

Cu 0.5616523506 1.3123205431 -1.5955322875

Cu -0.554883727 -1.1618473286 -0.6577770919

Cu 2.2264207286 -0.8259863697 0.2115148713

Cl 0.0171411805 -0.3823539964 -2.8999567255

Cl -1.1096460549 1.3723597953 2.6760049069

Cl 0.6391940294 -2.5582327096 0.619458825

Cl 3.9979371534 -1.8387588673 -0.3310598622

Cl 2.8254723254 0.9911429593 1.5456949508

C -4.4842540454 1.2040160548 1.0972121391

C -3.4722896819 0.8321109547 0.3074631925

H -4.7411831265 2.2525328304 1.2195633471

H -5.0969021023 0.4837331825 1.633655837

C -3.114230693 -0.5923242655 0.1676545222

C -2.6546603467 -1.0992405031 -1.0633864277

C -3.216956164 -1.487611085 1.2459891867

C -2.2673162326 -2.4504546072 -1.190586156

H -2.6834227935 -0.4740311654 -1.9535201052

C -2.9065276961 -2.8355787042 1.1045923848

H -3.5205940191 -1.0992827816 2.2153473922

C -2.4284822952 -3.3249379274 -0.1049807986

H -1.9866149744 -2.8355274506 -2.1697636766

H -3.0007233544 -3.500717719 1.9579611286

H -2.1418041461 -4.3676475495 -0.2051642375

Cl 0.7331665016 3.3472084361 -1.1338347725

C -2.6514999302 1.8251711712 -0.4589106724

H -1.5824293719 1.6997594279 -0.2347535958

H -2.7782556925 1.7331738214 -1.5469727572

H -2.910109483 2.850894754 -0.1831833287

TS1b

30

0 5

Cu 0.4355208022 -1.1592343763 -1.3031357388

O -0.5423066299 -0.0366807004 -0.1871121348

Cu -0.4731996967 1.6803813913 -0.9332885495

Cu -0.6414320022 -0.467962695 1.680609459

Cu -2.2975575454 -0.6191018694 -0.3781517918

Cl 0.1823085895 3.685165445 -0.5802798506

Cl 2.2990447437 -2.52073844 -1.097523836

Cl -2.8546318073 -1.0264031944 1.8418453704

Cl -2.7821424255 1.3915059286 -1.2908008638

Cl -1.3577624935 -2.5604862204 -1.3382999768

C 3.4965646683 -1.5236521888 0.3717793892

C 3.0669398315 -0.1893772971 0.6200393501

H 4.4285255719 -1.6370932301 -0.1762131687

H 3.3495209463 -2.2809806115 1.1368797165

C 2.0573622421 0.088028598 1.5858952051

C 1.7006927044 1.421727754 1.8961427701

C 1.3051974973 -0.9532983788 2.2338748705

C 0.6872821374 1.70083478 2.8052258476

H 2.190260373 2.249131309 1.3902878521

C 0.4434082839 -0.6705306939 3.3159873446

H 1.5525883258 -1.9953441534 2.0432601257

C 0.0633047143 0.6764157349 3.5263926746

H 0.3895707346 2.7329396631 2.9671518427

H 0.0651303208 -1.4623379816 3.9581013129

H -0.6765350941 0.9123256713 4.286278515

Cl 1.1826541518 0.6514668235 -2.3735398029

C 3.7268740746 0.9126824078 -0.1487479298

H 4.438785162 1.4607037782 0.4844566637

H 4.2798481166 0.50987672 -1.0023029906

H 3.0078878528 1.6371140162 -0.5477507854

cpx3b

30

0 5

Cu -0.712147499 -1.4774905054 0.3338921758

O 0.5414477868 -0.1336273838 0.594686549

Cu -0.2157313444 0.8423785565 1.9403189962

Cu 0.7328238202 1.4850417042 -0.5059766037

Cu 2.2728507515 -0.8338800658 0.1685026188

Cl 0.0310700441 2.9429674546 1.9395993108

Cl -2.6975289262 -2.5001500928 -0.4914851031

Cl 2.9693184083 1.2995707095 -0.3020807304

Cl 4.0698722817 -1.9458743056 0.3662615469

Cl 0.8098020143 -2.5680924562 -0.8256472829

C -3.4318867459 -0.9900324478 -1.4744363185

C -2.7586560941 0.2494356525 -1.1147130079

H -4.4755705641 -1.0353904953 -1.1629675956

H -3.315628666 -1.328897459 -2.5028831557

C -1.6020524753 0.6816778685 -1.8065541724

C -0.9549017379 1.9207842007 -1.4306505141

C -0.9800448667 -0.0875694529 -2.8191823895

C 0.1547940832 2.4057897323 -2.1681617834

H -1.5139565381 2.6392200794 -0.8345878553

C 0.1562078144 0.3629253985 -3.4867156369

H -1.3769879434 -1.0641151311 -3.0861639786

C 0.7169010757 1.597070733 -3.1913134996

H 0.4431276896 3.4525176019 -2.0906085624

H 0.6077981286 -0.2670681134 -4.2475898273

H 1.5929995801 1.9473561759 -3.7300426927

Cl -1.5775423547 -0.8613823817 2.4017448833

C -3.3623241224 1.0535077718 -0.0046540907

H -3.9455541544 1.9007366722 -0.3943380659

H -4.0349767283 0.4410765368 0.6044929344

H -2.6144653476 1.4787883727 0.6770094815

cpx4b

32

0 5

Cu -0.2417128611 -1.6680196823 0.267493441

O 0.5241117157 0.0877740681 0.3185264148

O -1.273366544 -3.1265715336 0.962948404

Cu 1.1853310323 -0.0358296736 2.0441639754

Cu 0.1083123355 1.8551559892 -0.1123613491

Cu 1.8213023964 -0.2898037816 -1.0619448065

Cl 0.6087244212 1.81452831 2.9619018531

Cl -3.5500218029 -2.0564820347 -1.1627469182

Cl 2.0399413164 2.1384486245 -1.14343086

Cl 3.6514371949 -0.8663397845 -1.9644027018

Cl 0.2585762275 -1.7840395013 -1.912665108

O -1.4507042757 -2.1153033335 1.7490789843

C -4.3376532333 -0.4975329261 -0.7189472073

C -3.4511648614 0.2578626201 0.217535344

H -5.2820193584 -0.7489343431 -0.2277451881

H -4.558918759 0.0357793239 -1.6444231642

C -2.5802701038 1.2173966097 -0.2458637792

C -1.8223792791 2.0430459808 0.6749557444

C -2.342872205 1.4550970752 -1.6514726457

C -1.2600283383 3.2595331035 0.2567977543

H -1.9018301053 1.8752866116 1.7443217823

C -1.5130033223 2.4542953713 -2.0603110701

H -2.789524912 0.7995564059 -2.3936220845

C -0.9172014022 3.3485038415 -1.1042877435

H -0.8907505097 3.9803776585 0.9824591628

H -1.2689683168 2.5779198482 -3.1105492519

H -0.3281210792 4.1889296397 -1.4604473689

Cl 1.9058699285 -2.0439503093 1.975621388

C -3.6318226796 -0.0914287627 1.6508803298

H -4.5353262738 0.3978298561 2.0437236357

H -3.7859501681 -1.172276672 1.748967231

H -2.7871591778 0.1760174005 2.2903078021

TS2b

32

0 5

Cu -0.2633999126 -1.6290659904 0.373289419

O 0.7671218151 -0.0149737129 0.2754888753

O -1.9403904116 -2.4184163696 0.8911894592

Cu 1.0839332404 0.2245317509 2.0881015115

Cu 0.1979921589 1.6633660632 -0.3353675046

Cu 2.2478554976 -0.5295196769 -0.8419745093

Cl 1.1657115982 2.3650468488 2.2803588648

Cl -2.1408992897 -1.7409547559 -2.2262389793

Cl 1.9141496717 1.6976586685 -1.7422232412

Cl 4.2538065992 -0.8932016622 -1.4287391835

Cl 1.2150359771 -2.6019571015 -0.9929774733

O -1.9936947628 -1.111499507 1.083742151

C -3.5431071644 -1.2521611396 -1.2178955447

C -3.2975154936 -0.1187545074 -0.2765087704

H -3.8069049005 -2.1375181336 -0.6291151435

H -4.3807316322 -1.0293512664 -1.8918602292

C -2.4907257122 1.0130546458 -0.6239493679

C -1.9474208621 1.8450576143 0.3978690681

C -2.2096589838 1.3620890796 -1.9741083602

C -1.2759957392 3.0371726669 0.0947382748

H -2.1226127399 1.5990343572 1.4430396546

C -1.4382737052 2.4602104204 -2.271636187

H -2.6227222671 0.7702953116 -2.7832605963

C -0.8995580449 3.2708209915 -1.2398682978

H -0.9455120375 3.6952450241 0.8931851366

H -1.2086330058 2.6995558308 -3.3055343008

H -0.3100711826 4.1478113041 -1.4903785109

Cl 0.8919764046 -1.7323939477 2.9060716696

C -4.3400225918 0.0000017209 0.7870003273

H -4.0403454112 0.675785847 1.5915485841

H -5.2620054505 0.4059093412 0.345694119

H -4.5705378616 -0.9762052256 1.2241511949

cpx5b

32

0 5

Cu 0.2782791137 -1.4730638854 -0.6500417834

O 1.0074306024 -0.0348409175 0.4016672909

O -1.1352201678 -2.6562506924 -0.8806668246

Cu 1.3647645326 -0.9793589589 1.940963493

Cu -0.1626552288 1.2619223658 1.0878789697

Cu 2.1262544443 0.746712361 -0.9393289811

Cl 0.6528845984 0.6772018167 3.2318823181

Cl -1.1408684533 0.1353379218 -2.7358973917

Cl 0.4947651397 2.6055218589 -0.5253264056

Cl 3.677417566 1.8276683837 -1.8874398606

Cl 2.1219978537 -1.3360886263 -1.9281918499

O -1.6318567009 -1.5734031927 -0.0665783272

C -2.5715668569 -0.8090537005 -2.2029424857

C -2.7333766443 -0.8589094024 -0.6943237434

H -2.4395964325 -1.8250571155 -2.5768468198

H -3.454917305 -0.3597094765 -2.6640157735

C -2.7251582294 0.5038644712 -0.0257707055

C -2.264384025 0.628201274 1.2955371314

C -3.1683529607 1.650405858 -0.6820035394

C -2.167706706 1.8961317805 1.9018826805

H -2.0513091988 -0.2667493006 1.8812024801

C -3.1044854997 2.9021042404 -0.074332839

H -3.5421985152 1.5855791629 -1.7005150871

C -2.593561199 3.0349437418 1.2076363693

H -1.9028729626 1.9646006181 2.9550291021

H -3.4381937853 3.779004223 -0.6210812983

H -2.5217624564 4.0124817085 1.6752407417

Cl 1.675292485 -3.0287819757 1.6647864995

C -3.9991048856 -1.6402115859 -0.3692111346

H -4.8844822147 -1.1415482794 -0.7787730883

H -3.9236788196 -2.6499481826 -0.7858786183

H -4.1148396984 -1.7209349439 0.7160036405

TS3b

32

0 5

Cu 0.7864407676 -1.0522637671 -1.2493876294

O 1.1708368842 -0.1928366499 0.3937664043

O -0.7170662664 -2.0635147868 -1.6308006493

Cu 1.5560316689 -1.7067702089 1.3741117902

Cu -0.5214733637 0.2468723159 1.0916787098

Cu 2.0347103986 1.40992438 -0.2122460804

Cl 0.0655741558 -1.2711250357 2.9288535147

Cl -1.1954120975 1.1425099952 -2.6202530873

Cl 0.0794593256 2.3859235327 0.8398443955

Cl 3.3686866475 3.0464532516 -0.3335569557

Cl 2.2963490206 0.2324560357 -2.2348684045

O -1.3231788441 -1.2192032222 -0.6194329588

C -2.47363674 -0.1038333298 -2.4586638919

C -2.592744018 -0.6756517979 -1.0570910297

H -2.2122390643 -0.9120098334 -3.1438643538

H -3.4234214792 0.3402378922 -2.7708242545

C -2.8806200142 0.3397674346 0.0334022499

C -2.6248570801 -0.0409198386 1.3731265982

C -3.357881704 1.6214184521 -0.2144085282

C -2.8135698663 0.8766046286 2.41925395

H -2.4710876123 -1.0925476988 1.6165656192

C -3.5582301145 2.5152162433 0.8356375759

H -3.5487174324 1.9533230034 -1.230609683

C -3.2660704136 2.1606668002 2.1477911831

H -2.6061448848 0.5631555767 3.4398650429

H -3.9205117027 3.515693123 0.6154471175

H -3.3970264183 2.8775876535 2.9524385798

Cl 2.6339144052 -3.0237916665 0.1398059322

C -3.6174647962 -1.8003298057 -1.0839857359

H -4.5920593843 -1.4274935979 -1.4175658883

H -3.2787959806 -2.5868768362 -1.7648738493

H -3.7359943964 -2.2338999334 -0.086854893

cpx6b

32

0 5

Cu 1.1071778759 -1.3485800069 -1.1133602856

O 1.0499982504 -0.1185604058 0.3459930775

O -0.4916931502 -2.2106863887 -0.81142178

Cu 1.3053210786 -1.3756674484 1.6868446378

Cu -0.7005675323 0.4617458968 0.6672485265

Cu 2.0786169299 1.3698643357 -0.217917426

Cl -0.1208440788 -0.6600693734 3.1375360739

Cl -0.9351189236 0.3623445779 -2.7436228767

Cl 0.0812319413 2.5381159018 0.4751625319

Cl 3.4973946489 2.9300588254 -0.3714461443

Cl 2.6931208387 -0.122371736 -2.0145351571

O -1.3405085101 -1.2692046545 -0.1487183643

C -2.2473831946 -0.8061540082 -2.3700549743

C -2.5459590749 -0.9393634502 -0.8884693987

H -1.9231709195 -1.7739268388 -2.7554414167

H -3.1429141634 -0.4869763634 -2.9104323299

C -2.9497108181 0.3532343567 -0.1927805706

C -2.8193477104 0.4124461145 1.2160702431

C -3.4281780068 1.4753038137 -0.8697741346

C -3.1346191555 1.5914377929 1.9060628894

H -2.628894036 -0.4954457241 1.7891550501

C -3.7447418843 2.6326780834 -0.1696703559

H -3.5296329413 1.4670384817 -1.9513941285

C -3.5802642016 2.7042206994 1.2128125082

H -3.0121435911 1.6178268573 2.9858241595

H -4.1029686114 3.501027291 -0.7158603909

H -3.8079553266 3.6246535432 1.741993322

Cl 2.5701403484 -2.8171328394 0.7385229484

C -3.5566705588 -2.0566422301 -0.6971408992

H -4.4816353221 -1.8448624872 -1.2447755912

H -3.1333869099 -3.000212626 -1.0562423026

H -3.7994910406 -2.1679273803 0.3633914792

cpx7b

34

0 5

Cu -0.610806 1.756989 -0.625293

O -0.941365 0.153749 0.289834

O 1.056180 2.084392 0.029890

Cu -0.611010 0.380590 2.149157

Cu 0.363774 -1.300477 0.492501

Cu -2.401686 -0.677890 -0.510821

Cl 0.131193 -1.564386 2.844877

Cl 4.976277 0.417087 -0.855022

Cl -1.349572 -2.636961 -0.471374

Cl -4.362899 -1.389121 -0.947571

Cl -2.607980 1.363847 -1.412081

O 1.524009 1.266944 1.068941

C 3.573889 1.369275 -0.139833

C 2.596591 0.442085 0.590779

H 4.033064 2.072352 0.558092

H 3.116638 1.913970 -0.966136

C 2.041804 -0.642214 -0.334188

C 2.166126 -2.042888 -0.008024

C 1.669945 -0.314216 -1.680492

C 2.066076 -3.017019 -1.040073

H 2.625254 -2.340153 0.932455

C 1.486947 -1.296241 -2.639848

H 1.521607 0.731782 -1.948187

C 1.716316 -2.657354 -2.329674

H 2.232068 -4.062416 -0.793194

H 1.179052 -1.011459 -3.642106

H 1.603905 -3.416296 -3.098443

Cl -1.394893 2.339982 2.333152

C 3.238788 -0.080787 1.863963

H 4.143122 -0.659036 1.647938

H 3.516392 0.776995 2.483059

H 2.545282 -0.694390 2.446517

Cl -0.073565 3.096783 -2.231745

Li 3.716901 -1.398643 -1.836591

TS4b

32

0 5

Cu 1.1266523702 -1.5326091061 -1.1060704441

O 1.2399686536 -0.1885245679 0.172048647

O -0.826493553 -1.7926931667 -0.8624771234

Cu 1.4872435279 -1.2959811133 1.6432147976

Cu -0.4150716238 0.5994222212 0.6799016555

Cu 2.3019742069 1.1823520574 -0.6470985012

Cl 0.5942486518 -0.1654113161 3.2122437222

Cl -4.4487251537 -0.4810898193 -2.5060442856

Cl 0.5403992786 2.5360833349 0.0917642824

Cl 3.9076238671 2.4909191313 -1.028957406

Cl 2.4445962027 -0.4474910571 -2.4673859702

O -1.2717059907 -1.2365556101 0.3894584788

C -2.1877083052 -1.1953083844 -1.5943881908

C -2.6247971909 -0.80023409 -0.1916414835

H -2.6141456509 -2.0766868993 -2.055752114

H -1.8264697958 -0.4315519116 -2.2799934102

C -2.669747171 0.6682897535 0.1805206983

C -2.3355274826 0.9786305003 1.5280826967

C -3.0149666609 1.7045843294 -0.6910444029

C -2.3811796351 2.3074547406 1.9791573361

H -2.2356629392 0.1806875487 2.2671579246

C -3.0425830106 3.0126249688 -0.2216531206

H -3.3124653735 1.4591274691 -1.7093527412

C -2.725674414 3.3210698856 1.1022197025

H -2.1284251175 2.5232361507 3.0138615185

H -3.317061233 3.8090116643 -0.9079946012

H -2.750938465 4.3520219547 1.4426269658

Cl 2.0261372216 -3.1053658896 0.5609519848

C -3.6905815595 -1.65378112 0.4352475325

H -4.656773405 -1.3847801156 -0.0000860411

H -3.4878176902 -2.7095403649 0.2286877918

H -3.7147306993 -1.5010898085 1.5188817111

cpx8b

32

0 5

Cu -0.8267403151 -1.2084404595 0.9944704574

O -0.9973979696 -0.0228028476 -0.4068654768

O -0.660785305 -2.4085783155 2.2289990978

Cu -1.1956412957 -1.1010864298 -1.9297805223

Cu 0.8733929409 0.3274091698 -0.6002420457

Cu -1.7338542905 1.6250741737 0.0948100494

Cl 0.1902441129 -0.1320088106 -3.2632585924

Cl 0.9599777102 0.5712208339 2.7869233162

Cl 0.3155890754 2.5191467717 -0.4994649226

Cl -3.0396971536 3.1668575311 0.6358114687

Cl -2.6186356879 -0.4026795999 1.8196104206

O 0.9252052764 -1.3842843538 0.3333090144

C 1.8934570098 -0.9487760909 2.539141935

C 2.1471131116 -1.2782926649 1.0747607477

H 1.2951215668 -1.7434140752 2.9926711586

H 2.8371416954 -0.8470319641 3.0826424104

C 2.9247909123 -0.1843576226 0.3316371164

C 2.9079356834 -0.2136399814 -1.0843283556

C 3.6410382409 0.8367540781 0.9656628468

C 3.5630524975 0.7798114249 -1.8270688392

H 2.5207477293 -1.0890040248 -1.6077338255

C 4.2821392131 1.8134185621 0.2179804187

H 3.674473476 0.8965568084 2.0493614866

C 4.2309742579 1.8019753198 -1.1770460543

H 3.5251701261 0.7377178925 -2.9122898012

H 4.8167647435 2.60819937 0.7311603869

H 4.7229581534 2.5847639627 -1.7467553354

Cl -2.2577104804 -2.8069924181 -1.2920285181

C 2.851994644 -2.6241321592 1.0194927433

H 3.8141496437 -2.5910116524 1.5434566089

H 2.2152420463 -3.3874131112 1.4816244638

H 3.029597631 -2.912509317 -0.0205878587

cpx7b_LiCl

34

0 5

Cu 0.890862931 -1.6649322862 -1.1824294939

O 1.7389557834 -0.2594476108 -0.1969720848

O -0.4876561879 -0.2163231707 -1.3601967673

Cu 1.247426237 -0.0751827786 1.5943502143

Cu 0.7248929395 1.2189053493 -0.8350342166

Cu 3.5071180979 -0.7812331702 -0.046872527

Cl 0.7675620646 2.0732805055 1.4430998029

Cl -4.7836389563 -1.2560273868 -1.0833729899

Cl 0.1951787918 2.8281689842 -2.1579816496

Cl 4.4986206074 0.3459341311 1.4196409914

Cl 3.1251644392 -2.4211344767 -1.4543746841

O -0.9390364245 -0.5881366036 -0.0307382755

C -2.9447893375 -1.3846541113 -1.061233461

C -2.3576194048 -0.5617047815 0.0912770196

H -2.711515035 -2.4477277855 -0.9596256014

H -2.6059508806 -1.0405313538 -2.0386593562

C -2.8655717266 0.8753141725 0.0589529897

C -3.5722613372 1.4314009253 1.1345873995

C -2.6909558607 1.6551692724 -1.0967253178

C -4.1247438649 2.7115113289 1.0456960606

H -3.7173705811 0.8572574692 2.045328018

C -3.2173550415 2.9454033416 -1.1754150603

H -2.1238484394 1.2628027946 -1.9361588707

C -3.9561129831 3.4710397965 -0.1139279858

H -4.6788277034 3.1168071801 1.8882268995

H -3.0319094394 3.535359003 -2.0690509551

H -4.3756957287 4.4711628887 -0.1793702046

Cl 1.1321065114 -1.980695371 2.4978972907

C -2.562272227 -1.2703892873 1.4194447259

H -3.6248157508 -1.4228485537 1.6359748946

H -2.0661833753 -2.2452395758 1.369937853

H -2.0999922995 -0.7081280648 2.2381066644

Cl -0.2983564312 -3.3370365202 -1.8566276079

Li -4.9753943867 1.1868197458 -0.7920537144

TS4b_LiCl

34

0 5

Cu 0.6053769684 -0.4676238634 -0.30602507

O -0.1887051688 -0.2175232112 1.4440284112

O 1.9643742801 0.8394013428 -0.0255858993

Cu 0.2852337312 1.3171423782 2.3786725551

Cu -0.1804863825 -1.3857435163 2.9015424187

Cu -2.0165772159 -0.3688042209 1.1139334499

Cl 0.8547816828 0.1019539157 4.2606672617

Cl 6.0426545367 -0.335941702 0.214524243

Cl -0.3168542819 -3.3865316848 2.2148484487

Cl -2.8172027315 -0.5539188199 3.0787206481

Cl -1.6625164483 -0.6793098522 -1.0119013336

O 2.2162495427 1.0857210718 1.3672166847

C 3.8779104055 0.3853859504 -0.0042674607

C 3.5936671607 0.6649265626 1.4767606166

H 4.1730276715 1.2105174154 -0.6430425448

H 3.6475465691 -0.5584297415 -0.4871754031

C 3.6744029782 -0.607205301 2.3058137594

C 4.4905483485 -0.7089444025 3.4361017379

C 2.960114154 -1.7387441392 1.8873347217

C 4.6186977112 -1.9233504494 4.1125885049

H 5.0529074611 0.1536843385 3.7822198891

C 3.0861480725 -2.9533010682 2.5605330918

H 2.307577834 -1.682993462 1.0163278126

C 3.9268342779 -3.0515115644 3.6711067592

H 5.2608292085 -1.9850125066 4.9872835889

H 2.5049591698 -3.8068660314 2.2205484547

H 4.0265511936 -3.9963903411 4.1982368686

Cl -0.8711965261 2.9235846385 1.6399814165

C 4.35600823 1.8457832837 2.0352974977

H 5.4288913568 1.6501592698 2.1075629304

H 4.198767687 2.7062536264 1.3788101237

H 3.9626706499 2.1008791386 3.0266397921

Cl 1.7350121517 -1.7555395794 -1.6338158322

Li 5.4048087216 -2.052021475 1.538854857

cpx7b_Cl

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-1 5

Cu 1.0538123072 -1.5338036056 -0.6348811689

O 1.3867237342 0.3009977374 -0.2009159871

O -0.7282378438 -0.751924677 -1.0216625994

Cu 0.624680143 0.8669751871 1.4068953981

Cu -0.0646239606 1.0324258763 -1.2402743681

Cu 3.2106372236 0.5368204614 -0.1681388266

Cl -0.2227740211 2.7086108679 0.5554826082

Cl -4.479193184 -2.7598854597 0.2476598908

Cl -0.8036368083 1.7633990007 -3.118031844

Cl 4.1092613855 2.3306430347 0.4495160381

Cl 3.4555289907 -1.5392320002 -0.8646837641

O -0.9728579147 -0.7984676246 0.406343204

C -2.7973419564 -2.2473636061 -0.1594123754

C -2.3692642254 -1.063996003 0.7067682216

H -2.1286339112 -3.0972687033 0.0090336362

H -2.7892675342 -2.0028701716 -1.2209158171

C -3.1765828586 0.1974887305 0.4597931134

C -3.6837405653 0.958171102 1.514771745

C -3.3619895495 0.6647679367 -0.8452477669

C -4.3524759582 2.1533315753 1.27552377

H -3.5602707892 0.6218811341 2.5408430274

C -4.0129919199 1.8687021606 -1.08414892

H -2.9687599006 0.1060233264 -1.6907694984

C -4.5133467075 2.6161137635 -0.0246205496

H -4.7384411186 2.729311549 2.1137079696

H -4.1098233518 2.224276571 -2.1069345102

H -5.0216104904 3.5594066009 -0.2115743619

Cl 1.2935881021 -0.3186552626 3.0355483232

C -2.2668959503 -1.4813725582 2.164181923

H -3.2576250492 -1.697317826 2.573899209

H -1.6428975787 -2.3787634913 2.2332320313

H -1.7884663309 -0.7006141096 2.7652571896

Cl 0.5761645922 -3.6375605167 -0.7256219409

TS4b_Cl

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-1 5

Cu -0.477889994 1.8502581518 -0.5259895829

O -0.8836192866 0.0387419048 -0.038520207

O 0.9458418381 1.9649498414 0.7761918675

Cu -0.1507696382 -0.7392444306 1.5132329542

Cu 0.0518491796 -1.2286032156 -1.1324063278

Cu -2.6079921836 -0.175013264 -0.7249709228

Cl -0.455618231 -2.7840091498 0.4425098549

Cl 5.0243191293 1.4879987698 -0.0574586125

Cl -0.6660176925 -0.4347830659 -3.026484567

Cl -4.0879103328 -1.6274013829 -1.0727211736

Cl -2.7976124512 2.041531637 -0.8141341269

O 1.170566649 0.7973562005 1.5882834819

C 2.6698887438 1.9233674036 0.4287939218

C 2.6016783395 0.6019805849 1.1729223291

H 2.998062444 2.8005209127 0.9723714205

H 2.6465625199 2.0251410024 -0.6469107353

C 2.6595074702 -0.6313155518 0.2960294718

C 3.03132711 -1.864915893 0.82653678

C 2.232967038 -0.5898237664 -1.0438380489

C 2.9894250676 -3.028839381 0.0593520467

H 3.3524749578 -1.9286768173 1.8620754866

C 2.1601147075 -1.7642428407 -1.8103430085

H 2.0550056622 0.3606685343 -1.5462348251

C 2.5594264854 -2.987167823 -1.2550138202

H 3.2868312952 -3.9727315841 0.5074595269

H 1.9442261739 -1.6859403517 -2.8741538447

H 2.5187630018 -3.8926850321 -1.8538628665

Cl 0.2842504767 -1.3791877128 3.5260466842

C 3.3788066858 0.5240312028 2.4648876928

H 4.4211290577 0.2630321427 2.2731828923

H 3.3455642379 1.4999073975 2.9574211176

H 2.9028137607 -0.2024907196 3.1340373482

Cl 0.3490687784 3.4748882962 -1.6889312075

TS5b

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Cu 0.0281546172 1.5535408866 0.142040853

Cl 0.0006047183 1.0709297544 2.4157294293

O -0.9440040944 -0.0795855234 -0.0739415498

C 3.519691505 1.2558958956 0.0686649628

O 1.3996007611 2.6588800304 -0.2552180763

Cu -1.2508262979 -0.8400816942 1.5938489175

Cu -0.7038411005 -1.0622143514 -1.62877973

Cu -2.6457580996 0.5746520643 -0.4674463326

C 2.9893196242 2.0548265442 1.2140064178

C 3.6131884065 -0.1506635829 0.137662433

C 4.0154002112 2.0201586913 -1.0936958416

O 2.2560048579 3.1500391214 0.770667579

Cl -3.5256184437 -0.1171503341 1.4716878975

Cl -0.4670135586 -2.8378254125 1.6927164275

Cl 1.3355075486 -0.9565038984 -2.2059135549

Cl -2.8179033378 -1.260034911 -2.138031419

Cl -1.689094287 2.4362186304 -1.27002587

H 2.4143400302 1.4528278614 1.9293493649

H 3.8692628502 2.4413690941 1.7614386392

C 4.4216297126 -0.8640631927 -0.7907210095

C 2.8569225932 -0.897806675 1.0840685079

H 3.9211817632 3.0935771228 -0.9278611578

H 5.0547324322 1.7590359429 -1.3250675626

H 3.4085051772 1.7554995002 -1.9703193065

C 4.507766086 -2.2348403917 -0.7386711622

H 4.9935729569 -0.3220064312 -1.537577792

C 2.9292104294 -2.2766521598 1.1095949227

H 2.1511502274 -0.4047239148 1.7494126721

C 3.7594041472 -2.9411770273 0.2098665221

H 5.1387581983 -2.7691478785 -1.4422437187

H 2.2980994013 -2.8303949891 1.7988461876

H 3.810412964 -4.0270197721 0.2310463497

cpx8b

32

0 5

Cu 0.8442247813 -0.6087550091 -1.1481021223

Cl 0.9839443068 1.4113202667 -2.0191181655

O -0.6657894842 -0.0147367034 -0.1915429014

C 3.4256949078 -0.618349675 0.2148289648

O 2.7921945499 -1.1210094408 -1.0720280739

Cu -0.1473044746 1.8000090868 0.1899942143

Cu -1.1642738104 -1.6113478244 0.6233213006

Cu -2.3907443942 0.3596179071 -0.8268841445

C 4.0025401676 0.4998564135 -0.6454174855

C 2.3596163058 -0.3388584841 1.2350043494

C 4.4609847502 -1.6307504823 0.6302631334

O 3.7113589028 -0.280558319 -1.8247894238

Cl -2.4913076381 2.1786264787 0.3774006321

Cl 0.589230818 3.8015054528 0.4962590806

Cl 0.1897084556 -2.7710116933 -0.7469611177

Cl -2.724798175 -1.6035072086 2.0261928837

Cl -3.0091772129 -1.1579254886 -2.1297769419

H 3.433853557 1.4378147812 -0.6617015302

H 5.0761687876 0.6862487774 -0.5462290893

C 1.7259081441 -1.4119632909 1.8712700641

C 1.9472508973 0.9622877804 1.5490969608

H 5.1555428027 -1.8103662548 -0.1955410898

H 5.0188906846 -1.2512189087 1.4933823778

H 4.0025593625 -2.5841212055 0.9063772564

C 0.6788207169 -1.1994315954 2.7643694689

H 2.0290595944 -2.4327571392 1.6495200057

C 0.9077500342 1.1783967768 2.4599709624

H 2.4552878088 1.8312479301 1.1356876642

C 0.2665671965 0.0963957702 3.0599378552

H 0.2017922857 -2.0467923604 3.2521261591

H 0.6515667986 2.1983368545 2.737761845

H -0.5569714272 0.2611768075 3.7495579075

TS5b

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Cu 0.8040631984 -0.6934411807 -1.0607452407

Cl 1.0521427946 1.2683029354 -2.0492907198

O -0.6966847762 0.029249044 -0.1875180812

C 3.3814376843 -0.7668716122 0.2177563512

O 2.6297425234 -1.3677216927 -0.8971570782

Cu -0.0735316495 1.8241403445 0.1321782395

Cu -1.3386254504 -1.5083801836 0.6459175378

Cu -2.3821487929 0.4809063263 -0.88089357

C 4.0290294307 0.3523013895 -0.5966881363

C 2.335091615 -0.4032609183 1.2466866467

C 4.4068854246 -1.7682790322 0.6980639853

O 4.1355219105 -0.3414222977 -1.8138985111

Cl -2.3925122206 2.3568898322 0.231582583

Cl 0.7718193575 3.7863215892 0.3870683597

Cl -0.0315418965 -2.7915097584 -0.6595042278

Cl -2.8555013821 -1.3464372126 2.0836494469

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H 3.4065615185 1.2514699016 -0.7000720978

H 5.0334080948 0.6156525203 -0.2297436555

C 1.6529328728 -1.4399307538 1.8965162014

C 1.9698944341 0.9210527622 1.5288250269

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H 4.960807755 -1.3571484066 1.5489765193

H 3.935509098 -2.7045888367 1.0086582037

C 0.6096865017 -1.1692338515 2.7779181766

H 1.9184697554 -2.474620041 1.6916717209

C 0.9341883777 1.1930774191 2.4264221063

H 2.5161164421 1.7607978215 1.1048599931

C 0.2450158095 0.1470259468 3.0420115872

H 0.0945457257 -1.9873638956 3.2767723495

H 0.7168177003 2.2271083587 2.6853597616

H -0.5769116061 0.3580672302 3.7208486243

cpx9b

32

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Cl -0.126866786 -0.2042239499 2.4691351197

Cl -0.8222518525 0.8101700739 -1.7263701132

Cl 0.8580660208 -2.8130586751 -0.5368720763

O 1.2738224806 -0.038065114 -0.0015019108

Cu 1.3929788097 1.3084230934 -1.247071841

Cu 2.5168030034 -1.3119211245 -0.4778392206

Cu 1.8489465232 0.6484045942 1.6046230521

Cl 1.8565176389 2.7485763715 0.5563769201

Cl 3.1127309786 0.1545867655 -2.2653098338

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H -4.4947362795 -2.4457960459 1.5490329815

C -3.5990169834 -0.974384644 0.1284824058

C -3.6147455931 0.5196697506 0.1690000759

C -3.4689729314 3.3143595103 0.1773307444

C -3.0044863476 1.2005727935 1.2279527922

C -4.1727543107 1.2647758492 -0.8734175321

C -4.1092540642 2.6517038317 -0.8634904156

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H -4.6523215468 0.7670322944 -1.7115461198

H -4.5471061523 3.2151986355 -1.6829690381

H -2.4095896449 3.090930499 2.0427978221

H -3.4019454339 4.3992352232 0.1732437902

O -2.177822163 -1.5365062753 -0.0043498593

O -2.4466434166 -2.4745355977 1.0726250602

C -4.3707636137 -1.6294027461 -0.9859591275

H -5.4349502048 -1.3801638716 -0.9128069988

H -3.9908633749 -1.3019452396 -1.9586124692

H -4.2531774527 -2.7149894208 -0.9231908493

TS5b

32

0 5

Cu -0.5037391324 -0.5835554515 -0.122232829

Cl -0.3231532351 -0.1519516408 2.3178958979

Cl -0.6052857362 1.3211047021 -1.660123562

Cl 0.6378714649 -2.6359060487 -0.9883337534

O 1.2709326905 -0.0443673887 -0.0310966466

Cu 1.6171755854 1.4149466806 -1.1008604476

Cu 2.4434875046 -1.3573187391 -0.5781058852

Cu 1.8081506693 0.4357824596 1.6629244689

Cl 2.2516038324 2.5787828617 0.8590456696

Cl 3.2811718142 0.2135829138 -2.159076848

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C -3.2782114508 -1.7782794417 1.4266562582

H -2.7904036477 -1.2072518372 2.2252321084

H -4.1754216874 -2.2881250489 1.8063318474

C -3.5393517442 -0.9939537153 0.1441925297

C -3.6294604698 0.5062583543 0.1681191724

C -3.6609409243 3.3005484036 0.0753360746

C -3.3122107537 1.2586209615 1.307029892

C -3.9451168624 1.181207552 -1.0225033007

C -3.9634265101 2.5665674714 -1.0659414662

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H -3.0431971479 0.7698376434 2.2383577415

H -4.1538603865 0.6195057924 -1.9285527812

H -4.1993388371 3.0734216669 -1.9972831327

H -3.1010236467 3.2137857337 2.1549166837

H -3.6679182182 4.3868712543 0.0418580664

O -2.2351416071 -1.2698504874 -0.478395137

O -2.3903034092 -2.7145831197 0.8530050116

C -4.5939128899 -1.6884446934 -0.6903107109

H -5.5905618477 -1.455446559 -0.3000422719

H -4.5434800377 -1.3790613887 -1.7367419125

H -4.4324674052 -2.7692782651 -0.653909593

cpx3c

32

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O -0.662853916 -0.0938162673 -0.1148180431

O 0.4722704245 1.4501948365 -3.5072351063

Cl 0.0511420343 2.5959867425 -0.6013651329

Cu -0.9506574675 1.3088017703 1.139759274

Cu 0.3594141129 -1.6334423234 0.2247160807

Cu -2.3764932063 -0.7505699894 -0.4270543417

O 1.5993698269 1.8734235962 -3.6358210155

Cl -0.454199039 2.3288059521 2.9557083132

Cl 1.3259931997 -1.1712010809 -1.9560263803

Cl -1.530301292 -2.9325722452 0.1468920756

Cl -3.0507362943 0.3612714154 1.449840924

Cl -2.3282068547 -0.0545476393 -2.5655510997

C 3.7754415329 1.2610146412 -0.4188306179

C 3.3156363479 0.9748298792 0.8092747954

H 4.0925243035 2.2705458459 -0.6687559706

H 3.7993082811 0.5225517486 -1.2177144749

C 2.851687842 -0.3899251804 1.1019907473

C 3.1744411987 2.0211918283 1.872604268

C 1.730095966 -0.5958732325 1.9383119063

C 3.4630639715 -1.5134287927 0.5230673305

H 3.5940241083 1.6850499949 2.8284684412

H 3.6844304895 2.940878374 1.5742576609

H 2.1214717732 2.2796127882 2.0560170399

C 1.206118826 -1.8779044178 2.1450416194

H 1.2711655473 0.2520684269 2.4498119086

C 2.8927404422 -2.7687915081 0.6434354467

H 4.3639727684 -1.3797571986 -0.0691219694

C 1.7215034861 -2.958482313 1.4010241914

H 0.3705139015 -2.0229714246 2.8284028114

H 3.3350837772 -3.6172636228 0.1289289662

H 1.2965593061 -3.9511033979 1.5226076399

TS1c

32

0 5

Cu -0.6486524252 -1.3444021667 -0.3693968586

O 0.8092444981 -0.1371081959 -0.2749540157

O -2.0432933425 -2.6640369981 -0.4448680097

Cl -0.2843910369 -1.6494481361 1.849194255

Cu 1.2790838678 0.1283214821 1.5373940493

Cu 0.1020807905 1.3145976979 -1.2818447575

Cu 2.3651336628 -1.0185220821 -0.7718913539

O -3.1723360962 -2.6051736004 0.1259258468

Cl 1.1384052789 1.3004865858 3.3161594787

Cl -1.2791680245 -0.2531791121 -2.2757306421

Cl 1.8340267092 2.5195080967 -1.6321280086

Cl 3.5211419677 -0.0735773505 0.8303943059

Cl 1.5906926667 -2.6315570185 -1.9090912152

C -4.1476054904 -0.9759815501 0.2706150711

C -3.4998901318 -0.023086427 1.0833070572

H -4.9422885671 -1.5763025046 0.7076285313

H -4.218875182 -0.8149838481 -0.8035960139

C -2.8320617881 1.1124471145 0.4792461027

C -3.4334603109 -0.2481081078 2.553076629

C -1.6908911287 1.6705303975 1.0917068945

C -3.2745695197 1.6634603733 -0.7441782928

H -3.5715863179 0.6833716175 3.1126292866

H -4.1825383215 -0.9766777057 2.8753233728

H -2.4484425842 -0.652482249 2.8342885019

C -0.9257536087 2.6170948351 0.4202964977

H -1.3524175958 1.3206935557 2.0668435527

C -2.5527553302 2.6555577564 -1.3791927991

H -4.1968422554 1.3057959176 -1.1947170061

C -1.3277034702 3.084596889 -0.8473874653

H -0.0280956077 3.0177744771 0.890477165

H -2.9051757005 3.0641991546 -2.3218646672

H -0.7655986057 3.8834611019 -1.3253484923

cpx4c

32

0 5

Cu -0.562691811 0.9682976213 -1.1567174071

O 0.9101290228 -0.0625515354 -0.4771748376

O -2.0592573866 2.02518843 -1.3553710884

Cl -1.3456982044 -1.0804775706 -1.8262952678

Cu 0.2253184858 -1.8362022099 -0.3053505901

Cu 1.5280015426 1.0996016234 0.852713179

Cu 2.6845415003 -0.4274729376 -0.9410881903

O -3.1758786933 1.3319886589 -1.8278620224

Cl -0.7372485367 -3.5120180798 0.6272333842

Cl 0.4817124676 2.805517473 -0.1052597647

Cl 2.2118083819 0.0276092486 2.5410134286

Cl 2.4386532536 -2.5823961881 -0.7962355592

Cl 3.7863969446 1.3730736664 -0.9107877683

C -4.2298509651 1.4247495461 -0.8681308623

C -3.9005102042 0.2535159684 -0.0096162436

H -5.1609060319 1.2737697587 -1.4237159048

H -4.2395565671 2.4100173175 -0.3960714951

C -2.9594726706 0.3612114985 1.0347728645

C -4.5020122972 -1.0187551448 -0.4609753973

C -2.4444865448 -0.7981218186 1.6868462684

C -2.4724353953 1.63318874 1.4539979179

H -5.5787566905 -0.9972245041 -0.232807615

H -4.419346128 -1.0799655564 -1.5533360972

H -4.0639434712 -1.9214555243 -0.0359211266

C -1.5133561705 -0.6869685904 2.6939463536

H -2.7398197643 -1.7936532312 1.3709790093

C -1.5529989182 1.7321182423 2.4813398033

H -2.8085775395 2.5388238938 0.9642440184

C -1.0766412511 0.579091353 3.1043248901

H -1.0996879528 -1.5846454893 3.1453013545

H -1.1891350385 2.7089538575 2.7867814801

H -0.3419333364 0.6586147331 3.9016191056