Supporting Information

Selective Formation of α -Alkylidene Cyclic Carbonates via Carboxylative Cyclization of Propargyl Alcohols in Supercritical Carbon Dioxide

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General information:

All reactions were performed under an atmosphere of argon using standard Schlenk techniques. Solvents were dried by standard procedures and freshly distilled under argon. Liquefied carbon dioxide (99.999%) was used as received without further purification. Tri-*n*-butylphosphine and 2-methyl-3-propyn-2-ol (**1a**) were used after purification by distillation under argon. 2-methyl-3-propyne-2-ol (**1l**) was prepared by using a procedure similar to one reported in the literature.¹ Other internal propargyl alcohols (**1b-1k** and **1m-1o**) were prepared by Sonogashira reaction of terminal alcohols with aryl halides according to the literature methods.²

NMR chemical shifts were referenced to residual protio impurities in the deuterated solvent (¹H) or the deuterated solvent (¹³C). Abbreviations for NMR data are as follows: s = singlet, d = doublet, q = quartet, or m = multiplet.

NMR data for 1.

2-Methyl-4-phenyl-3-butyn-2-ol (**1b**)

¹H NMR (300.5 MHz, CDCl₃) δ 1.60 (s, 6H, C(CH₃)₂), 2.17 (s, 1H, OH), 7.27 (m, 3H, C₆H₅), 7.40 (m, 2H, C₆H₅); ¹³C NMR(75.5 MHz, CDCl₃) δ 31.3, 65.3, 81.9, 93.9, 122.7, 127.97, 127.80, 131.4.

2-Methyl-4-(4'-chloro)phenyl-3-butyn-2-ol (**1c**)

¹H NMR (300.5 MHz, CDCl₃) δ 1.60 (s, 6H, C(CH₃)₂), 2.17 (s, 1H, OH), 7.28 (m, 4H, C₆H₄); ¹³C NMR(75.5 MHz, CDCl₃) δ 31.4, 65.6, 81.0, 94.7, 121.2, 128.5, 132.8, 134.2.

2-Methyl-4-(4'-acetyl)phenyl-3-butyn-2-ol (**1d**)

^1H NMR (300.5 MHz, CDCl_3) δ 1.59 (s, 6H, $\text{C}(\text{CH}_3)_2$), 2.54 (s, 3H, COCH_3), 2.42 (s, 1H, OH), 7.42 (m, 2H, C_6H_4), 7.83 (m, 2H, C_6H_4); ^{13}C NMR(75.5 MHz, CDCl_3) δ 26.5, 31.3, 65.5, 81.3, 97.2, 127.7, 128.1, 131.7, 136.1, 197.4.

2-Methyl-4-(4'-cyano)phenyl-3-butyn-2-ol (**1e**)

^1H NMR (300.5 MHz, CDCl_3) δ 1.59 (s, 6H, $\text{C}(\text{CH}_3)_2$), 2.18 (s, 1H, OH), 7.50 (m, 2H, C_6H_4), 7.55 (m, 2H, C_6H_4); ^{13}C NMR(75.5 MHz, CDCl_3) δ 31.2, 65.6, 80.6, 98.2, 111.6, 118.4, 127.7, 131.9, 132.1.

2-Methyl-4-(4'-nitro)phenyl-3-butyn-2-ol (**1f**)

^1H NMR (300.5 MHz, CDCl_3) δ 1.67 (s, 6H, $\text{C}(\text{CH}_3)_2$), 1.92 (s, 1H, OH), 7.53 (m, 2H, C_6H_4), 8.15 (m, 2H, C_6H_4); ^{13}C NMR(75.5 MHz, CDCl_3) δ 31.2, 65.6, 80.4, 99.0, 123.5, 129.66, 129.67, 132.3

2-Methyl-4-(4'-trifluoromethyl)phenyl-3-butyn-2-ol (**1g**)

^1H NMR (300.5 MHz, CDCl_3) δ 1.61 (s, 6H, $\text{C}(\text{CH}_3)_2$), 2.02 (s, 1H, OH), 7.51 (m, 4H, C_6H_4); ^{13}C NMR(75.5 MHz, CDCl_3) δ 31.3, 65.6, 80.9, 96.2, 103.5, 125.2 (q, $^3J_{\text{C-F}} = 3.8$ Hz), 125.9 (q, $^1J_{\text{C-F}} = 583$ Hz), 126.6 (q, $^2J_{\text{C-F}} = 69$ Hz), 131.9.

2-Methyl-4-(4'-methyl)phenyl-3-butyn-2-ol (**1h**)

^1H NMR (300.5 MHz, CDCl_3) δ 1.59(s, 6H, $\text{C}(\text{CH}_3)_2$), 1.91 (s, 1H, OH), 2.34 (s, 3H, PhCH_3), 7.08 (m, 2H, C_6H_4), 7.29 (m, 2H, C_6H_4); ^{13}C NMR(75.5 MHz, CDCl_3) δ 21.4, 31.5, 65.6, 82.2, 93.0, 119.6, 129.0, 131.5, 138.3

2-Methyl-4-(4'-methoxy)phenyl-3-butyn-2-ol (**1i**)

^1H NMR (300.5 MHz, CDCl_3) δ 1.59 (s, 6H, $\text{C}(\text{CH}_3)_2$), 1.92 (s, 1H, OH), 3.78(s, 3H, OCH_3), 6.80 (m, 2H, C_6H_4), 7.33 (m, 2H, C_6H_4); ^{13}C NMR(75.5 MHz, CDCl_3) δ 31.6, 55.2, 65.6, 82.0, 92.4, 103.5, 113.9, 114.8, 133.0.

2-Methyl-4-(2'-naphthyl)-3-butyn-2-ol (**1j**)

^1H NMR (300.5 MHz, CDCl_3) δ 1.65 (s, 6H, $\text{C}(\text{CH}_3)_2$), 2.02 (s, 1H, OH), 7.46 (m, 3H, C_{10}H_7), 7.76 (m, 3H, C_{10}H_7), 7.93 (s, 1H, C_{10}H_7); ^{13}C NMR(75.5 MHz, CDCl_3) δ 31.6, 65.7, 82.5, 94.0, 120.0, 126.5, 126.6, 127.69, 127.71, 127.9, 128.4, 131.5, 132.7, 132.9.

2-Methyl-4-(2'-pyridyl)-3-butyn-2-ol (**1k**)

^1H NMR (300.5 MHz, CDCl_3) δ 1.61 (s, 6H, $\text{C}(\text{CH}_3)_2$), 3.38 (s, 1H, OH), 7.17 (m, 1H, Py), 7.36 (m, 1H, Py), 7.59 (m, 1H, Py), 8.51 (m, 1H, Py); ^{13}C NMR(75.5 MHz, CDCl_3) δ 31.2, 65.2, 81.2, 94.2, 122.8, 127.0, 136.2, 142.9, 149.7.

1-Phenylethynylcyclohexane-1-ol (**1m**)

^1H NMR (300.5 MHz, CDCl_3) δ 1.2–1.3 (s, 1H, $\text{C}(\text{CH}_2)_5$), 1.5–2.1 (s, 10H, $\text{C}(\text{CH}_2)_5$ and OH), 7.28 (m, 3H, C_6H_5), 7.41 (m, 2H, C_6H_5); ^{13}C NMR(75.5 MHz, CDCl_3) δ 24.4, 25.2, 40.0, 69.1, 84.3, 92.8, 122.9, 128.15, 128.20, 131.6.

4-(4'-Nitro)phenyl-3-butyn-2-ol (**1n**)

^1H NMR NMR (300.5 MHz, CDCl_3) δ 1.55 (d, $^2J_{\text{H-H}} = 6.6$ Hz, 3H, CHCH_3), 2.05 (s, 1H, OH), 4.77(q, $^2J_{\text{H-H}} = 6.6$ Hz, 1H, CHCH_3), 7.53 (m, 2H, C_6H_4), 8.15 (m, 2H, C_6H_4); ^{13}C NMR(75.5 MHz, CDCl_3) δ 24.1, 58.8, 82.2, 96.2, 123.5, 129.5, 132.4, 147.2.

3-(4'-Nitro)phenyl-2-propyn-1-ol (**1o**)

^1H NMR NMR (300.5 MHz, CDCl_3) δ 1.80 (s, 1H, OH), 4.52 (s, 2H, CH_2), 7.53 (m, 2H, C_6H_4), 8.15 (m, 2H, C_6H_4); ^{13}C NMR(75.5 MHz, CDCl_3) δ 51.5, 83.8, 92.5, 123.5, 129.4, 132.4, 147.2.

Characterization data for 2.

(*Z*)-4-Benzylidene-5,5-dimethyl-1,3-dioxolan-2-one (**2b**).

According to the procedure for the preparation of **2d**, **2b** was obtained as a white solid (776 mg, 76%) after purification by column chromatography and Kugelrohr distillation: mp 40-42 °C; ¹H NMR (300.5 MHz, CDCl₃) δ 1.62 (s, 6H, C(CH₃)₂), 5.49 (s, 1H, C=CH), 7.20-7.40 (m, 3H, C₆H₅), 7.50-7.56 (m, 2H, C₆H₅); ¹³C NMR (75.6 MHz, CDCl₃) δ 27.6, 85.5, 101.5, 127.5, 128.4, 128.6, 132.3, 150.6, 151.2; Anal. Calcd for C₁₂H₁₂O₃: C, 70.57; H, 5.92. Found: C, 70.45; H, 6.12.

(*Z*)-4-(4'-Chloro)benzylidene-5,5-dimethyl-1,3-dioxolan-2-one (**2c**).

According to the procedure for the preparation of **2d**, **2c** was obtained as a white powder (953 mg, 80%) after purification by column chromatography and Kugelrohr distillation: mp 110-111 °C; ¹H NMR (300.5 MHz, CDCl₃) δ 1.66 (s, 6H, C(CH₃)₂), 5.44 (s, 1H, C=CH), 7.28 (A₂B₂ pattern, 2H, C₆H₄), 7.44 (A₂B₂ pattern, 2H, C₆H₄); ¹³C NMR (75.6 MHz, CDCl₃) δ 27.6, 85.6, 100.4, 128.7, 129.6, 130.9, 133.2, 151.1; Anal. Calcd for C₁₂H₁₁ClO₃: C, 60.39; H, 4.65; Cl, 14.85. Found: C, 60.11; H, 4.82; Cl, 14.96.

(*Z*)-4-(4'-Cyano)benzylidene-5,5-dimethyl-1,3-dioxolan-2-one (**2e**).

According to the procedure for the preparation of **2d**, **2e** was obtained as a yellow solid (983 mg, 86%) after purification by column chromatography and Kugelrohr distillation: mp 170-171 °C; ¹H NMR (300.5 MHz, CDCl₃) δ 1.70 (s, 6H, C(CH₃)₂), 5.50 (s, 1H, C=CH), 7.61 (m, 4H, C₆H₄); ¹³C NMR (75.6 MHz, CDCl₃) δ 27.6, 85.6, 100.0, 110.7, 118.7, 128.8, 132.3, 137.0, 150.5, 153.7; Anal. Calcd for C₁₃H₁₁N₁O₃: C, 68.11; H, 4.84; N, 6.11. Found: C, 68.18; H, 4.71; N, 5.99.

(*Z*)-5-(4'-Nitro)benzylidene-4,4-dimethyl-1,3-dioxolan-2-one (**2f**).

According to the procedure for the preparation of **2d**, **2f** was obtained as a yellow powder (965mg, 77%) after purification by column chromatography and Kugelrohr distillation: mp 155-157 °C; ^1H NMR (300.5 MHz, CDCl_3) δ 1.71 (s, 6H, $\text{C}(\text{CH}_3)_2$), 5.56 (s, 1H, $\text{C}=\text{CH}$), 7.67 (A_2B_2 pattern, 2H, C_6H_4), 7.92 (A_2B_2 pattern, 2H, C_6H_4); ^{13}C NMR (75.6 MHz, CDCl_3) δ 27.6, 85.8, 99.7, 123.9, 129.0, 139.0, 146.5, 150.4, 154.2; Anal. Calcd for $\text{C}_{12}\text{H}_{11}\text{N}_1\text{O}_5$: C, 57.83; H, 4.45; N, 5.62. Found: C, 57.63; H, 4.46; N, 5.57.

(*Z*)-5-(4'-Trifluoromethyl)benzylidene-4,4-dimethyl-1,3-dioxolan-2-one (**2g**).

According to the procedure for the preparation of **2d**, **2g** was obtained as a white powder (1.179 g, 87%) after purification by column chromatography and Kugelrohr distillation: mp 85-87 °C; ^1H NMR (300.5 MHz, CDCl_3) δ 1.69 (s, 6H, $\text{C}(\text{CH}_3)_2$), 5.53 (s, 1H, $\text{C}=\text{CH}$), 7.59 (A_2B_2 pattern, 4H, C_6H_4); ^{13}C NMR (75.6 MHz, CDCl_3) δ 27.5, 85.7, 100.2, 110.7, 124.0 (q, $^1J_{\text{C-F}} = 271.6$ Hz), 125.4 (q, $^2J_{\text{C-F}} = 3.8$ Hz), 128.5, 136.0, 150.8, 152.7; Anal. Calcd for $\text{C}_{13}\text{H}_{11}\text{F}_3\text{O}_3$: C, 57.36; H, 4.07; F, 20.94. Found: C, 57.40; H, 4.16; F, 20.95.

(*Z*)-5-(4'-Methyl)benzylidene-4,4-dimethyl-1,3-dioxolan-2-one (**2h**).

According to the procedure for the preparation of **2d**, **2h** was obtained as a white powder (681mg, 62%) after purification by column chromatography and Kugelrohr distillation: mp 69-70 °C; ^1H NMR (300.5 MHz, CDCl_3) δ 1.66 (s, 6H, $\text{C}(\text{CH}_3)_2$), 2.33(s, 3H, $\text{C}_6\text{H}_4\text{CH}_3$), 5.45 (s, 1H, $\text{C}=\text{CH}$), 7.14 (A_2B_2 pattern, 2H, C_6H_4), 7.42 (A_2B_2 pattern, 2H, C_6H_4); ^{13}C NMR (75.6 MHz, CDCl_3) δ 21.2, 27.7, 85.5, 128.3, 129.3, 129.5, 137.5, 149.9; Anal. Calcd for $\text{C}_{13}\text{H}_{14}\text{O}_3$: C, 71.54; H, 6.47. Found: C, 71.61; H, 6.55.

(*Z*)-5-(2'-Naphthyl)methylidene-4,4-dimethyl-1,3-dioxolan-2-one (**2j**).

According to the procedure for the preparation of **2d**, **2j** was obtained as a white powder (913 mg, 72%) after purification by column chromatography: mp 140-141 °C; ¹H NMR (300.5 MHz, CDCl₃) δ 1.72 (s, 6H, C(CH₃)₂), 5.64 (s, 1H, C=CH), 7.45–7.94 (m, 7H, naphthyl); ¹³C NMR (75.6 MHz, CDCl₃) δ 27.8, 85.6, 101.7, 126.1, 126.4, 127.6, 127.7, 128.1, 128.3, 129.9, 132.5, 133.4, 151.0, 151.3; Anal. Calcd for C₁₆H₁₄O₃: C, 75.57; H, 5.55. Found: C, 75.71; H, 5.37.

(Z)-5-(2'-Pyridyl)methylidene-4,4-dimethyl-1,3-dioxolan-2-one (**2k**).

According to the procedure for the preparation of **2d**, **2k** was obtained as a yellow solid (623 mg, 64%) after purification by column chromatography and Kugelrohr distillation: mp 85-86 °C; ¹H NMR (300.5 MHz, CDCl₃) δ 1.69 (s, 6H, C(CH₃)₂), 5.78 (s, 1H, C=CH), 7.13 (m, 1H, pyridyl), 7.67 (m, 1H, pyridyl), 7.83 (m, 1H, pyridyl), 8.53 (m, 1H, pyridyl); ¹³C NMR (75.6 MHz, CDCl₃) δ 27.6, 85.8, 103.0, 122.0, 123.5, 136.6, 149.4, 150.8, 152.0, 153.5; Anal. Calcd for C₁₁H₁₁O₃N: C, 64.38; H, 5.40; N, 6.83. Found: C, 64.20; H, 5.25; N, 6.82.

(Z)-5-Benzylidene-1,3-dioxaspiro[4.5]decan-2-one (**2m**).

According to the procedure for the preparation of **2d**, **2m** was obtained as a white powder (908 mg, 74%) after purification by column chromatography: mp 143-144 °C; ¹H NMR (300.5 MHz, CDCl₃) δ 1.3-1.5 (m, 1H), 1.6-1.9 (m, 7H), 2.0-2.2 (m, 2H), 5.47 (s, 1H, C=CH), 7.2-7.4 (m, 3H, phenyl), 7.53 (d, 2H, phenyl); ¹³C NMR (75.6 MHz, CDCl₃) δ 21.7, 24.3, 36.6, 87.3, 101.7, 127.4, 128.4, 128.6, 132.5, 150.9, 151.4; Anal. Calcd for C₁₅H₁₆O₃: C, 73.75; H, 6.60. Found: C, 73.79; H, 6.71.

X-ray Structure Determination of 2d.

Colorless platelet crystals of **2d** of an adequate quality for X-ray measurements were grown from a CH₂Cl₂/pentane solution of the crude compounds at –30 °C. A single crystal of approximate dimensions of 0.15×0.15×0.15 mm was mounted on a glass fiber. All measurements were made on a Rigaku Saturn CCD area detector with a graphite-monochromatized Mo-*K*α source ($\lambda = 0.71070$ Å). Indexing was performed from 7 images that were exposed for 3 seconds. The crystal-to-detector distance was 45.05 mm. The data were collected at a temperature of -80 ± 1 °C to a maximum 2θ value of 54.9°. A total of 720 oscillation images were collected. A sweep of data was carried out using ω scans from –110.0 to 70.0° in 0.5° steps, at $\chi = 45.0^\circ$ and $\phi = 0.0^\circ$. A second sweep was performed using ω scans from –110.0 to 70.0° in 0.5° steps, at $\chi = 45.0^\circ$ and $\phi = 90.0^\circ$. The exposure rate was 3.0 s/°, and the detector swing angle was –19.86°. Readout was performed in the 0.070 mm pixel mode. Of the 9545 reflections collected, 2677 were unique ($R_{\text{int}} = 0.058$); equivalent reflections were merged. The data were collected for Lorentz and polarization effects as well as absorption.

All calculations were performed using the CrystalStructure crystallographic software package. The heavy atom positions were determined by a direct program method (SIR92), and the remaining non-hydrogen atoms were found by subsequent Fourier techniques (DIRDIF99). All of the non-hydrogen atoms were refined anisotropically. In the final cycles of refinement, hydrogen atoms were located at idealized positions ($d(\text{C-H}) = 0.95$ Å) with isotropic thermal parameters, and were included in calculations without refinement of their parameters. The function minimized in least-squares was $\Sigma w(F_o^2 - F_c^2)^2$ ($w = 1/[\sigma^2(F_o^2)]$). The final R1 and wR2 ($R1 = \Sigma[|F_o| - |F_c|]/\Sigma|F_o|$ and $wR2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{0.5}$) values were 0.057 and 0.203, respectively.

Figure 1 Structure of **2d** determined by X-ray crystallography with 50% thermal ellipsoids. Selected bond distances (Å) and angles (deg): C(1)–O(1) 1.320(3), C(1)–O(2) 1.365(3), C(1)–O(3) 1.187(3), C(2)–O(1) 1.467(3), C(3)–O(2) 1.390(3), C(3)–C(6) 1.313(3), C(6)–C(7) 1.473(3), C(6)–C(3)–O(2) 125.4(2), C(3)–C(6)–C(7) 131.9(2), C(7)–C(6)–C(3)–O(2) –0.8(4).

References

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- (2) (a) Sabourin, E. T.; Onopchenko, A. *J. Org. Chem.* **1983**, 48, 5135-5137. (b) Mal'kina, A. G.; Brandsma, L.; Vasilevsky, S. F.; Trofimov, B. A. *Synthesis*, **1996**, 589-590.

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2b

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2b

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Real Imag (F2)
 Real Imag (F1)
 Data from (F2) 143
 Data from (F1) 322
 Data from (F2) 145
 Data from (F1) 320
 High Inten Clip 1149.783263
 Low Inten Clip 30.000000
 Zero Level 0.000000
 Slice Post 1
 Slice Post 1
 WDM 15

1.6631
 5.4430
 7.2400
 7.2694
 7.2917
 7.4285
 7.4569

2c

Date : Sun Oct 9 15:54:38 2005

Filename	Loading ID: radata
Comment	1H S/N
SliceHistory	noisy
Exphase	BCN
IrrMode	
Points (F2)	512 points
Points (F1)	512 points
SamplingPoints (F2)	512 points
SamplingPoints (F1)	512 points
Freq (F2)	600.00 Hz
Freq (F1)	600.00 Hz
Resol (F2)	15.62 Hz
Resol (F1)	15.62 Hz
ScanTimes	32 times
DummyTimes	4 times
AcqTime	64.0000 msec
PulseDelay	1.0000 sec
RecircGain	19
ObsNucleus	1H
ObsFreq	300.40 MHz
ObsOffset	130750.00 Hz
Solvent	CDCl3
Temperature	23.2 C
SpinnerSpeed	19 Hz
RealFreq (F2)	RealPart
RealFreq (F1)	RealPart
DataFrom (F2)	146
DataFrom (F1)	329
DataTo (F2)	145
DataTo (F1)	328
HighIntenClip	600.000000
LowIntenClip	60.000000
ZeroLevel	0.000000
SlicePos	1
SlicePost	1
NAME	16

1.4152
1.6850
1.6850
2.1921
2.1921
5.5315
5.5315

7.9159
7.6866
7.6023
7.5747
7.2400

2d

Date: Tue Sep 5 10:47:37 2006
 Filename: LoadingID.mdata
 Comment: 00-57905-185/00137.r
 SliceHistory: not
 ExpDate: 30M
 Del's: 32758 points
 SamplingRate: 32758 points
 Freq: 300.0 MHz
 Resol: 0.24 Hz
 AcqTime: 6.01 sec
 DataTime: 0.11 sec
 Acquisition: 4095.000 MHz
 PulseProgram: 16
 Review: 16
 Processing: 300.00 MHz
 Observed: 130.00 MHz
 TossTime: 10 Hz
 Solvent: CDCl3
 Temperature: 24.1 C
 SpinningSpeed: 10 Hz
 Realtime: 24.1 C
 DataRate: 10 Hz
 DataTime: 21.216
 HighIntensity: 633.785025
 LowIntensity: -40.785156
 WNO: 2
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2d

Date: Tue Dec 27 19:55:35 2005

Filename: CarbAc20.mn
 Comment: p-acetylphenyl-card
 SliceHistory: none
 ExpMode: none
 IrrMode: BOM

Points (F2): 512 points
 Points (F1): 512 points
 SamplingPoints (F1): 512 points
 Freq (F2): 8000.0 Hz
 Freq (F1): 8000.0 Hz
 Resol (F2): 15.62 Hz
 Resol (F1): 15.62 Hz

Scans: 64 times
 Dummy: 4 times
 AcqTime: 54.0000 sec
 PulseSeq: 1
 RecieverGain: 25

ObsNucleus: 1H
 ObsFreq: 300.40 MHz
 ObsOffset: 130780.00 Hz

Solvent: CDCl3
 Temperature: 22.9 C
 SpinnerSpeed: 16 Hz

RealPart: 150
 RealPart: 311

Data from (F2): 151
 Data from (F1): 312

HighIntenClip: 1246.021484
 LowIntenClip: 50.000000
 ZeroLevel: 0.000000
 SlicePos: 1
 SlicePos: 1

NOE: 15

Date: Thu Feb 5 11:32:02 2004

File Name: Loading10.mdata

Comment: 37-40128-2 CDCl3/10/14

Sample Name:

ExpDate:

Points: 32768 points

SamplingRate: 32768 points

Freq: 500.0 Hz

Resol: 0.24 Hz

ScanTime: 32 Lines

DwellTime: 0 Lines

AcqTime: 4056.0000 sec

PulseDelay: 1.0000 sec

ReceiverGain: 1.0

ObsNucleus: ¹H

ObsFreq: 300.40 MHz

ObsOffset: 130780.00 Hz

Solvent: CDCl3

Temperature: 22.1 C

SpinnerSpeed: 16 Hz

RealPart: RealPart

Data: Data

Gain: 2.00

HighResolution: 632.45445

LowResolution: -40.55205

WDW: EM

SSB: 0.0

GB: 90.0

BF: 100.0

CF: 0.15 Hz

W5: 0.00 Hz

W6: 0.30 Hz

W7: 0.00 Hz

W8: 0.00 Hz

W9: 0.00 Hz

W10: 0.00 Hz

W11: 0.00 Hz

W12: 0.00 Hz

W13: 0.00 Hz

W14: 0.00 Hz

W15: 0.00 Hz

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5656
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2277

5.3048

7.6591
7.6088
7.5609
7.5400

S21

Date: Wed Nov 10 15:47:35 2004

Filename: Loading ID: ncdat1

Comment: NO2-carbonate/CDCl₃/rt

ExpMode: run

ExpMode: 80M

Points: 32768 points

SamplingPoints: 32768 points

Freq: 8000.0 Hz

Resol: 0.24 Hz

ScanTime: 54 lines

AcqTime: 0 lines

PulseDelay: 4056.0000 msec

RecycleGain: 1.0000 sec

22

ObsNucleus: ¹H

ObsFreq: 300.40 MHz

ObsOffset: 130780.00 Hz

Solvent: CDCl₃

Temperature: 22.7 °C

SpinProgram: 16 Hz

RealPart: 18909

DataFrom: 21215

DataTo: 928.133484

HighIntenClip: -94.620728

LowIntenClip: 2

NOESY: 0.0 %

T1: 90.0 %

T2: 100.0 %

T3: 0.15 Hz

T4: 0.00 Hz

GF: 0.00 %

WS: 0.00 %

WP: 0.00 %

pp: 0 point

2f

157.24
155.13
149.91
148.81
98.82
96.82
76.82
99.56
29.58
27.77
27.22
32.22
37.22
55.00
95.56
27.60

Date : Wed Nov 10 17:48:39 2004
Filename Loading10.mdata
Comment NO2-carbonate/CDCl3/rt/
Slicehistory bcm
ExpMode BCM
IrrMode
Points 32768 points
SamplingPoints 32768 points
Freq 25000.0 Hz
Resol 0.75 Hz
ScanTime 1000 times
DwellTime 0 times
AcqTime 1310.7200 msec
PulseDelay 5.0000 sec
RecircGain 30
ObsNucleus ¹³C
ObsFreq 75.45 MHz
ObsOffset 126064.52 Hz
Solvent CDCl3
Temperature 23.9 C
Spinnerspeed 15 Hz
RealImag RealPart
DataFrom 1
Datafo 32768
HighIntenClip 115.594467
LowIntenClip -13.934219
WIDM0 2
T1 0.0 s
T2 90.0 s
T3 100.0 s
T4 6.15 Hz
GF 0.00 Hz
CF 0.00 Hz
KS 0.00 s
MP 0.00 s
PP 0 point

2f

100

2

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612

614

Date: Sat Nov 19 12:54:49 2005

File Name: LoadingF10.mdata

Content: 1H 5/N

SliceHistory: none

ExpMode: none

InnMode: none

Points (F2): 512 points

Points (F1): 512 points

SamplingPoints (F2): 512 points

SamplingPoints (F1): 512 points

Freq (F2): 8000.0 Hz

Freq (F1): 8000.0 Hz

Resol (F2): 15.62 Hz

Resol (F1): 15.62 Hz

ScanTimes: 32 times

Quantities: 4 times

AcqTime: 64.0000 msec

Pulsedelay: 1.0000 sec

RecieverGain: 18

ObsNuc1: 1H

ObsF1: 300.40 MHz

ObsF2: 130.780 00 MHz

Solvent: CDCl3

Temperature: 21.5 C

SpinnerSpeed: 16 Hz

RealMag (F2): RealPart

RealMag (F1): RealPart

Data (F2): 143

Data (F1): 328

Data (F2): 142

Data (F1): 325

HighlightedClip: 1000.000000

LowIntenClip: 150.000000

ZeroLevel: 0.000000

SlicePos: 1

SlicePos: 1

WIND: 16

Date: Sat Sep 3 14:30:25 2005
 Filename: loading10.mdata
 Content: 08-53063-181/DEC13/r.1
 SliceH: 5.00
 ExpMode: 1H
 PPM: 30M
 Points: 32768 points
 SamplingPoints: 32768 points
 Freq: 300.0 MHz
 Resol: 0.24 Hz
 Scans: 8 times
 DummyTimes: 0 times
 AcqTime: 4055.0000 msec
 PulseDelay: 1.0000 sec
 RecycleGain: 15
 ObsNucleus: ¹H
 ObsFreq: 300.40 MHz
 ObsP1sec: 130.780.00 Hz
 Solvent: CDCl₃
 Temperature: 22.3 °C
 SpinningSpeed: 16 Hz
 RealPart: 1907
 DataFram: 21217
 Data: 0
 HighIntenClis: 730.356329
 LowIntenClis: -47.332166
 WNOVD: 2
 T1: 0.0 s
 T2: 0.0 s
 T3: 0.0 s
 T4: 160.0 s
 BF: 0.15 Hz
 CF: 0.00 Hz
 NS: 0.00 s
 MS: 0.00 s
 AP: 16921 points

2h

Date: Sat Sep 3 14:25:33 2005
 Filename: LoadingID.mvdat2
 Content: 38-53942-181/2DC13/r.t
 SliceHistory:
 ExpMode: bco
 IrrMode: bco

Points: 32768 points
 SamplingPoints: 32768 points
 Freq: 25000.0 Hz
 Prg: C-75 Hz

Scans: 56 times
 DwellTime: 0 times
 AcqTime: 1312.7200 sec
 PulseDelay: 1.0000 sec
 Recycle: 30

ObsNucleus: ¹³C
 ObsFreq: 75.45 MHz
 ObsOffset: 128364.52 Hz

Solvent: CDCl3
 Temperature: 23.9 C
 SolvrSpeed: 16 Hz

RealPart: 6824
 DataFCS: 26534
 Data0: 375.451019
 HighIntenClip: -51.175291
 LowIntenClip:

NOVO
 T1: 2
 T2: 0.0 s
 T3: 90.0 s
 T4: 100.0 s
 T5: C-75 Hz
 T6: C-00 Hz
 T7: C-00 Hz
 T8: C-00 Hz
 T9: 13934 point

21

Date	Wed Oct 6 14:00:09 2004
Filename	LoadingFID.mdata
Comment	37-4082 -f /CDE13/r/t/H
SlicerHistory	
ExpMode	non
IntMode	BCM
Points	32768 points
SamplingPoints	32768 points
Freq	8000.0 Hz
Resol	0.24 Hz
ScanTimes	15 times
QueryTimes	0 times
AcqTime	4095.0000 msec
PulseDelay	1.0000 sec
RetrievalGain	1b
ObsNuc1Leop	1H
ObsFreq	300.40 MHz
ObsOffset	130750.00 Hz
Solvent	CDC13
Temperature	23.8 C
SpinnerSpeed	14 Hz
RealImag	RealPart
ImagDataFrac	8507
ImagDataGain	21217
HighIntenClip	896.875831
LowIntenClip	-59.017751
NOHD	2
1	0.0 x
2	90.0 x
3	105.0 x
4	0.15 Hz
5	0.00 Hz
6	0.00 x
7	0.00 x
8	0.00 x
9	0.00 x
10	0.00 x

Date : Wed Oct 6 15:07:21 2004

Filebase LoadingID nedate
 Comment 37-4052 -7 /CIX13/ci/13
 SliceHistory
 ExpMode Oca
 IrrMode BCM

Points 32768 points
 SamplingPoints 32768 points
 Freq 25000.0 Hz
 Resol 0.76 Hz

Scanlines 500 times
 DummyTimes 0 times
 AcqTime 1310.7200 msec
 PulseDelay 5.0000 sec
 RecivGain 30

ObsNucleus ¹³C
 ObsFreq 75.45 MHz
 ObsOffset 125054.52 Hz

Solvent CDCl₃
 Temperature 24.4 C
 SpinnerSpeed 17 Hz

RealPart
 DataProc 6825
 DataTo 25535
 HighIntenClip 154.745582
 LowIntenClip -16.098831

WDW 2
 T1 0.0 s
 T2 90.0 s
 T3 100.0 s
 T4 0.15 Hz
 GF 0.00 Hz
 WS 0.00 s
 BP 0.00 s
 PP 0 point

2k

Date : Sat Nov 19 08 43:30 2005

Filename : LoadingF10.mdata
 Comment : 1H 5/N
 SliceHistory : messy
 ExpMode : BCK
 IrrMode :

Points (F2) : 512 points
 Points (F1) : 512 points
 SamplingPoints (F2) : 512 points
 SamplingPoints (F1) : 512 points
 Freq (F2) : 8000.0 Hz
 Freq (F1) : 8000.0 Hz
 Reso (F2) : 15.62 Hz
 Reso (F1) : 15.62 Hz

ScanTimes : 68 times
 DwellTimes : 4 times
 AcqTime : 54.0000 msec
 PulseDelay : 1.0000 sec
 RecycleGain : 19

ObsNucleus : 1H
 ObsFreq : 300.40 MHz
 ObsOffset : 130780.00 Hz

Solvent : CDCl3
 Temperature : 21.3 C
 SpinnSpeed : 10 Hz

RealPart : RealPart
 RealPart : 145
 DataFrom (F2) : 327
 DataTo (F2) : 144
 DataFrom (F1) : 321
 DataTo (F1) : 2000.000000
 HighIntenClip : 100.000003
 LowIntenClip : 0.000000
 ZeroLevel : 1
 SlicePos : 1
 SlicePos : 1

NOVO

15

0.847
0.855
1.736
1.729
7.013
7.223
7.453

7.546
7.528
7.369
7.343
7.317
7.263
7.240

2m

Date : Wed Nov 2 17:25:00 2005

Filename : LoadingfID.neddata
Comment : 08-51101-125/CDCl3/r.t.

SliceHistory :
ExpMode : non
IrrMode : BCM

Points : 32768 points
SamplingPoints : 32768 points
Freq : 8000.0 Hz
Resol : 0.24 Hz

ScanTimes : 8 times
DumTimes : 0 times
AcqTime : 4095.0000 msec
PulseDelay : 1.0000 sec
RecieverGain : 15

ObsNucleus : ¹H
ObsFreq : 300.40 MHz
ObsOffset : 130750.00 Hz

Solvent : CDCl3
Temperature : 22.0 C
SpinnerSpeed : 10 Hz

RealPart :
DataFrom : 8913
DataTo : 21223
HighIntenClip : 92.211876
LowIntenClip : -5.933950

NAME : 2
T1 : 0.0 s
T2 : 90.0 s
T3 : 100.0 s
T4 : 0.15 Hz
BF : 0.00 Hz
GF : 0.00 s
MS : 0.00 s
WDW : 14243 point

Date: Wed Nov 2 17:31:36 2005

 Filename: LoadingID.mdata
 Comment: 08-51101-125/CDC13/r.t.

 SliceHistory
 ExpMode
 ProcMode
bco
BCH
 Points: 32768 points
 SamplingPoints: 32768 points
 Freq: 25000.0 Hz
 Resol: 0.76 Hz

 Scans: 107 times
 DummyTimes: 0 times
 AcqTime: 1310.7200 msec
 PulseDelay: 1.0000 sec
 RecircGain: 30

 ObsNucleus: ¹³C
 ObsFreq: 75.45 MHz
 ObsOffset: 125064.52 Hz

 Solvent: CDCl₃
 Temperature: 22.9 C
 SpinnSpeed: 14 Hz

 RealPart: 6820
 DataFrom: 26630
 DataTo: 533.277161
 HighIntenClip: -51.028625

 WIDOW: 2
 T1: 0.0 s
 T2: 0.0 s
 T3: 90.0 s
 T4: 100.0 s
 BF: 0.15 Hz
 CF: 0.00 Hz
 W5: 0.00 s
 W6: 0.00 s
 PP: 13896 point

2m

Date: Thu Nov 3 09:06:14 2005

Filename: LoadingF10.mdata
 Comment: 1H 5/N
 SliceHistory: none
 ExpMode: EOM
 IrrMode: EOM

Points (F2): 512 points
 Points (F1): 512 points
 SamplingPoints (F2): 512 points
 SamplingPoints (F1): 512 points
 Freq (F2): 8000.0 Hz
 Freq (F1): 8000.0 Hz
 Resol (F2): 15.62 Hz
 Resol (F1): 15.62 Hz

Scans: 96 times
 DummyTimes: 4 times
 AcqTime: 64.0000 msec
 PulseDelay: 1.0000 sec
 RecycleGain: 20

ObsNucleus: 1H
 ObsFreq: 300.40 MHz
 ObsOffset: 130780.00 Hz

Solvent: CDCl3
 Temperature: 21.8 C
 SpinnerSpeed: 13 Hz

RealImag (F2): RealPart
 RealImag (F1): RealPart
 DataFrom (F2): 147
 DataFrom (F1): 330
 DataFrom (F1): 142
 DataFrom (F1): 328
 HighIntenClip: 185.000000
 LowIntenClip: 18.000000
 ZeroLevel: 0.000000
 SlicePos: 1
 SlicePos: 1
 WID: 16