| Compounds for derivatization formula, CAS #, purity, amount, type of packaging, price in US \$ | Structure | <mark>δ ²H (or δ D)</mark> (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements) | δ ¹³ C (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements) |
|---|------------------|--|---|
| Acetic anhydride #1, $C_4H_6O_3$, CAS # 108-24-7, 99.5 %, ca. 1 mL sealed under argon in glass ampoule, US \$250. | | -133.2 ± 2.1 ‰ from -131.5 to -136.0 ‰ n = 4 | -20.98 ± 0.03 ‰ from -20.94 to -21.01 ‰ n = 4 |
| Acetic anhydride #2, $C_4H_6O_3$, CAS # 108-24-7, 99.5 %, ca. 1 mL sealed under argon in glass ampoule, US \$250. | | -200.5 ± 1.5 ‰ from -198.5 to -202.5 ‰ n = 10 | -38.65 ± 0.01 ‰ from -38.64 to -38.65 ‰ n = 5 |
| Methanol, CH ₃ OH, 99.8 %, anhydrous, CAS # 67-56-1, the δ^2 H values characterize: (1) bulk hydrogen; (2) methyl hydrogen (calculated after subtracting the OH-hydrogen that was liberated in reactions between MeOH and Na metal). δ^{13} C was determined in bulk methanol. 5 mL sealed in glass ampoule, US \$250. | Н Н—С—ОН Н | bulk methanol: -112.6 ± 0.8 ‰ from -111.8 to -113.5 ‰ n = 3 methyl hydrogen: -141 ± 3 ‰ from -138 to -143 ‰ n = 3 | - 46.77 ± 0.04 ‰ from -46.74 to -46.82 ‰ n = 3 |
| Phthalic acid #2, $C_8H_6O_4$, CAS # 88-99- 3, δ^2H measured in Na-phthalate to exclude carboxyl hydrogen. $\delta^{13}C$ measured in free acid. 3 g in glass vial, US \$250 | HO OH | - 81.9 ± 1.2 ‰ from -81.8 to -83.0 ‰ n = 4 | - 29.98 ± 0.01 ‰ from -29.96 to -29.99 ‰ n = 3 |