The uploaded metadata consists of raw 1 H-NMR files used in the experimental analysis from "Metal Catalysis Acting on Nitriles in Early Earth Hydrothermal Systems". Three datasets are provided: standards used during analysis, spectra from nitrile reactions at 90°C, and spectra from nitrile reactions at 20°C. Data was originally generated with the MestReNova software and provided as MNOVA files. Additional files with the chemical shifts (ppm, δ) and intensities for each spectra are provided as Excel files. For the Excel file sheets, labelling is as follows:

AN= acetonitrile

MN= malononitrile

SF= sodium formate

H2= hydrogen gas (H₂)

Catalysts are listed as their elemental symbol or molecular formula.